

Dodecane, 1,12-dibromo-

Other names:	1,12-Dibromododecane Dodecamethylene dibromide
Inchi:	InChI=1S/C12H24Br2/c13-11-9-7-5-3-1-2-4-6-8-10-12-14/h1-12H2
InchiKey:	ZJJATABWMGVVRZ-UHFFFAOYSA-N
Formula:	C12H24Br2
SMILES:	BrCCCCCCCCCCCCBr
Mol. weight [g/mol]:	328.13
CAS:	3344-70-5

Physical Properties

Property code	Value	Unit	Source
gf	78.80	kJ/mol	Joback Method
hf	-238.35	kJ/mol	Joback Method
hfus	37.41	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.677		Crippen Method
mcvol	214.940	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	1946.00		NIST Webbook
tb	606.28	K	Joback Method
tc	793.23	K	Joback Method
tf	344.60	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.98	J/mol×K	606.28	Joback Method
cpg	524.31	J/mol×K	637.44	Joback Method
cpg	538.89	J/mol×K	668.60	Joback Method
cpg	552.74	J/mol×K	699.75	Joback Method
cpg	565.92	J/mol×K	730.91	Joback Method
cpg	578.44	J/mol×K	762.07	Joback Method

cpg	590.36	J/mol×K	793.23	Joback Method
cpl	457.38	J/mol×K	354.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	433.39	J/mol×K	312.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	434.17	J/mol×K	313.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	434.98	J/mol×K	315.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	435.79	J/mol×K	316.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	436.62	J/mol×K	318.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	437.46	J/mol×K	319.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	438.31	J/mol×K	321.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	439.17	J/mol×K	322.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	440.04	J/mol×K	324.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	440.91	J/mol×K	325.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	441.80	J/mol×K	327.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	442.68	J/mol×K	328.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	443.57	J/mol×K	330.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	444.47	J/mol×K	331.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	432.62	J/mol×K	310.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	446.26	J/mol×K	334.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	447.15	J/mol×K	336.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	448.04	J/mol×K	337.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	448.93	J/mol×K	339.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	449.82	J/mol×K	340.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	450.69	J/mol×K	342.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	451.57	J/mol×K	343.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	452.43	J/mol×K	345.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	453.29	J/mol×K	346.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	454.13	J/mol×K	348.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	454.96	J/mol×K	349.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	455.78	J/mol×K	351.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	456.59	J/mol×K	352.65	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
cpl	445.36	J/mol×K	333.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K

cpl	457.90	J/mol×K	355.15	Heat Capacity of alpha,omega-Bromochloroalkanes and ?,?-Dibromoalkanes: Their Dependence on the Hydrocarbon Chain Length and Temperature (285.15 to 355.15) K
dvisc	0.0023816	Pa×s	344.60	Joback Method
dvisc	0.0001921	Pa×s	606.28	Joback Method
dvisc	0.0007332	Pa×s	431.83	Joback Method
dvisc	0.0004784	Pa×s	475.44	Joback Method
dvisc	0.0003354	Pa×s	519.05	Joback Method
dvisc	0.0002484	Pa×s	562.67	Joback Method
dvisc	0.0012368	Pa×s	388.21	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	488.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.72197e+01
Coeff. B	-5.92693e+03
Coeff. C	-1.06880e+02
Temperature range (K), min.	456.92
Temperature range (K), max.	604.60

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Heat Capacity of
alpha,omega-Bromochloroalkanes and
Joback Method
1,2-dibromoalkanes: Their Dependence
on the Hydrocarbon Chain Length and
Temperature (285.15 to 355.15) K:
McGowan Method:

NIST Webbook:

The Yaws Handbook of Vapor
Pressure:

<https://www.doi.org/10.1021/je201002j>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3344705&Units=SI>

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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