

Dodecane, 1-iodo-

Other names:	1-Iodododecane Dodecyl iodide Lauryl iodide n-Dodecyl iodide
Inchi:	InChI=1S/C12H25I/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-12H2,1H3
InchiKey:	GCDPERPXPRESHJF-UHFFFAOYSA-N
Formula:	C12H25I
SMILES:	CCCCCCCCCCCCI
Mol. weight [g/mol]:	296.23
CAS:	4292-19-7

Physical Properties

Property code	Value	Unit	Source
gf	108.28	kJ/mol	Joback Method
hf	-214.14	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	79.90	kJ/mol	NIST Webbook
log10ws	-5.79		Crippen Method
logp	5.342		Crippen Method
mcvol	205.760	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	1635.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1644.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1922.00		NIST Webbook
ripol	1953.00		NIST Webbook
tb	571.40	K	NIST Webbook
tc	753.68	K	Joback Method
tf	283.06	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.03	J/molxK	753.68	Joback Method
cpg	477.26	J/molxK	567.10	Joback Method
cpg	493.73	J/molxK	598.20	Joback Method
cpg	509.42	J/molxK	629.29	Joback Method
cpg	524.37	J/molxK	660.39	Joback Method
cpg	538.60	J/molxK	691.49	Joback Method
cpg	552.14	J/molxK	722.58	Joback Method
dvisc	0.0002084	Paxs	567.10	Joback Method
dvisc	0.0049982	Paxs	283.06	Joback Method
dvisc	0.0020139	Paxs	330.40	Joback Method
dvisc	0.0010191	Paxs	377.74	Joback Method
dvisc	0.0006002	Paxs	425.08	Joback Method
dvisc	0.0003930	Paxs	472.42	Joback Method
dvisc	0.0002780	Paxs	519.76	Joback Method
hvapt	63.50	kJ/mol	531.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	432.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49414e+01
Coeff. B	-4.86646e+03
Coeff. C	-9.99850e+01
Temperature range (K), min.	432.08
Temperature range (K), max.	605.33

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4292197&Units=SI
The Yaws Handbook of Vapor Pressure: Crippen Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	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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