

DECANE, 1,2-DIBROMO-

Other names:	1,2-Dibromodecane
Inchi:	InChI=1S/C10H20Br2/c1-2-3-4-5-6-7-8-10(12)9-11/h10H,2-9H2,1H3
InchiKey:	XBRBOTTWTQOCJH-UHFFFAOYSA-N
Formula:	C10H20Br2
SMILES:	CCCCCCCCC(Br)CBr
Mol. weight [g/mol]:	300.08
CAS:	28467-71-2

Physical Properties

Property code	Value	Unit	Source
af	0.6574		Cheméo Relay (1.0)
gf	59.52	kJ/mol	Joback Method
hf	-225.92	kJ/mol	Cheméo Relay (1.0)
hfus	28.70	kJ/mol	Joback Method
hvap	68.44	kJ/mol	Cheméo Relay (1.0)
ie	9.93	eV	Cheméo Relay (1.0)
log10ws	-5.93		Cheméo Relay (1.0)
logp	4.895		Crippen Method
mcvol	186.760	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
tb	530.92	K	Cheméo Relay (1.0)
tc	733.18	K	Cheméo Relay (1.0)
tf	266.04	K	Cheméo Relay (1.0)
vc	0.684	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.66	J/mol×K	560.08	Joback Method
cpg	486.62	J/mol×K	755.21	Joback Method
cpg	475.59	J/mol×K	722.69	Joback Method
cpg	463.96	J/mol×K	690.17	Joback Method
cpg	451.69	J/mol×K	657.65	Joback Method
cpg	438.74	J/mol×K	625.12	Joback Method

cpg	425.07	J/mol×K	592.60	Joback Method
dvisc	0.0006056	Pa×s	433.57	Joback Method
dvisc	0.0002299	Pa×s	560.08	Joback Method
dvisc	0.0003012	Pa×s	517.91	Joback Method
dvisc	0.0004141	Pa×s	475.74	Joback Method
dvisc	0.0035444	Pa×s	307.06	Joback Method
dvisc	0.0009613	Pa×s	391.40	Joback Method
dvisc	0.0017060	Pa×s	349.23	Joback Method
hvapt	67.00	kJ/mol	446.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54516e+01
Coeff. B	-4.73524e+03
Coeff. C	-8.67640e+01
Temperature range (K), min.	399.03
Temperature range (K), max.	553.74

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28467712&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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