1,16-Dibromohexadecane

Other names: Hexadecane, 1,16-dibromo-
Inchi: InChI=1S/C16H32Br2/c17-15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-16-18/h1-16H2
InchiKey: OTFBUFWEFKVFFR-UHFFFAOYSA-N
Formula: C16H32Br2
SMILES: BrCCCCCCCCCCCCCCCCBr
Mol. weight [g/mol]: 384.23
CAS: 45223-18-5

Physical Properties

Property code	Value	Unit	Source
gf	112.48	kJ/mol	Joback Method
hf	-320.91	kJ/mol	Joback Method
hfus	47.77	kJ/mol	Joback Method
hvap	64.08	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	7.238		Crippen Method
mcvol	271.300	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
tb	697.80	K	Joback Method
tc	879.68	K	Joback Method
tf	389.68	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.64	J/mol×K	697.80	Joback Method
cpg	740.82	J/mol×K	728.11	Joback Method
cpg	757.18	J/mol×K	758.43	Joback Method
cpg	772.75	J/mol×K	788.74	Joback Method
cpg	787.57	J/mol×K	819.05	Joback Method
cpg	801.70	J/mol×K	849.37	Joback Method
cpg	815.17	J/mol×K	879.68	Joback Method
dvisc	0.0016844	Pa×s	389.68	Joback Method

dvisc	0.0008256	Pa×s	441.03	Joback Method
dvisc	0.0004695	Pa×s	492.39	Joback Method
dvisc	0.0002971	Pa×s	543.74	Joback Method
dvisc	0.0002034	Pa×s	595.09	Joback Method
dvisc	0.0001479	Pa×s	646.45	Joback Method
dvisc	0.0001127	Pa×s	697.80	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.75772e+01
Coeff. B	-6.59355e+03
Coeff. C	-1.23560e+02
Temperature range (K), min.	504.92
Temperature range (K), max.	661.12

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C45223185&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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