Dicyclohexano-18-crown-6

Other names:	Dibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin, eicosahydro-
	Dicyclohexo-18-crown-6
	Dicyclohexyl-18-crown-6
	Dicyclohexyl-18-crown-6 ether
	Perhydrodibenzo-18-crown-6
	2,5,8,15,18,21-Hexaoxatricyclo[20.4.0.0(9,14)]hexacosane
	Dicyclohexano-18-crown-6 ether
	Crown ether dicyclohexyl-18-crown-6
	NSC 252171
	2,3,11,12-Dicyclohexano-1,4,7-10,13,16-hexaoxacyclooctadecane
	cis-Dicyclohexano-18-crown-6
	DCH-18-crown-6
	icosahydrodibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin
Inchi:	InChI=1S/C20H36O6/c1-2-6-18-17(5-1)23-13-9-21-11-15-25-19-7-3-4-8-20(19)26-16-12-
InchiKey:	BBGKDYHZQOSNMU-UHFFFAOYSA-N
Formula:	C20H36O6
SMILES:	C1CCC2OCCOCCOC3CCCCC3OCCOCCOC2C1
Mol. weight [g/mol]:	372.50
CAS:	16069-36-6

Physical Properties

Property code	Value	Unit	Source
gf	-430.36	kJ/mol	Joback Method
hf	-1154.79	kJ/mol	Joback Method
hfus	55.21	kJ/mol	Joback Method
hvap	89.53	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.722		Crippen Method
mcvol	295.300	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
tb	906.84	K	Joback Method
tc	1176.76	K	Joback Method
tf	464.32	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.10	J/mol×K	906.84	Joback Method
cpg	1174.82	J/mol×K	1131.77	Joback Method
cpg	1168.35	J/mol×K	1086.79	Joback Method
cpg	1157.81	J/mol×K	1041.80	Joback Method
cpg	1143.23	J/mol×K	996.81	Joback Method
cpg	1124.64	J/mol×K	951.83	Joback Method
cpg	1177.19	J/mol×K	1176.76	Joback Method
dvisc	0.0000027	Pa×s	906.84	Joback Method
dvisc	0.0000046	Pa×s	833.09	Joback Method
dvisc	0.0000086	Pa×s	759.33	Joback Method
dvisc	0.0000183	Pa×s	685.58	Joback Method
dvisc	0.0000473	Pa×s	611.83	Joback Method
dvisc	0.0001581	Pa×s	538.07	Joback Method
dvisc	0.0007755	Pa×s	464.32	Joback Method

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=C16069366&Units=SI
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume