

Di-cyclohexadiene

Inchi:	InChI=1S/C12H16/c1-2-4-12-10-7-5-9(6-8-10)11(12)3-1/h1,3,5,7,9-12H,2,4,6,8H2
InchiKey:	OPOFYMSEXICFOW-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	C1=CC2C3C=CC(CC3)C2CC1
Mol. weight [g/mol]:	160.26
CAS:	2808-38-0

Physical Properties

Property code	Value	Unit	Source
chl	-7035.00 ± 7.10	kJ/mol	NIST Webbook
gf	248.32	kJ/mol	Joback Method
hf	4.13	kJ/mol	Joback Method
hfus	18.46	kJ/mol	Joback Method
hvap	42.84	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.165		Crippen Method
mvol	138.760	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
tb	500.64	K	Joback Method
tc	729.20	K	Joback Method
tf	265.54	K	Joback Method
vc	0.525	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.98	J/molxK	500.64	Joback Method
cpg	356.96	J/molxK	538.73	Joback Method
cpg	377.33	J/molxK	576.83	Joback Method
cpg	396.21	J/molxK	614.92	Joback Method
cpg	413.70	J/molxK	653.02	Joback Method
cpg	429.90	J/molxK	691.11	Joback Method
cpg	444.92	J/molxK	729.20	Joback Method
dvisc	0.0011498	Paxs	265.54	Joback Method

dvisc	0.0010988	Paxs	304.72	Joback Method
dvisc	0.0010609	Paxs	343.91	Joback Method
dvisc	0.0010317	Paxs	383.09	Joback Method
dvisc	0.0010086	Paxs	422.27	Joback Method
dvisc	0.0009897	Paxs	461.46	Joback Method
dvisc	0.0009741	Paxs	500.64	Joback Method

Sources

Crippen Method:	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2808380&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
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

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