1,2-Dihexylcyclopropene

Other names: Cyclopropene, 1,2-dihexyl-
Inchi: InChI=1S/C15H28/c1-3-5-7-9-11-14-13-15(14)12-10-8-6-4-2/h3-13H2,1-2H3
InchiKey: OTAPPAKLMIEBOQ-UHFFFAOYSA-N
Formula: C15H28
SMILES: CCCCCCC1=C(CCCCCC)C1
Mol. weight [g/mol]: 208.38
CAS: 35365-52-7

Physical Properties

Property code	Value	Unit	Source
chl	-9445.60	kJ/mol	NIST Webbook
chs	-9058.00	kJ/mol	NIST Webbook
gf	154.58	kJ/mol	Joback Method
hf	-224.95	kJ/mol	Joback Method
hfus	32.11	kJ/mol	Joback Method
hvap	50.82	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.627		Crippen Method
mcvol	207.050	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
tb	563.13	K	Joback Method
tc	735.72	K	Joback Method
tf	306.79	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.86	J/mol×K	563.13	Joback Method
cpg	545.61	J/mol×K	591.90	Joback Method
cpg	562.56	J/mol×K	620.66	Joback Method
cpg	578.75	J/mol×K	649.43	Joback Method
cpg	594.23	J/mol×K	678.19	Joback Method
cpg	609.02	J/mol×K	706.96	Joback Method

cpg	623.16	J/mol×K	735.72	Joback Method
dvisc	0.0020928	Pa×s	306.79	Joback Method
dvisc	0.0012686	Pa×s	349.51	Joback Method
dvisc	0.0008576	Pa×s	392.24	Joback Method
dvisc	0.0006261	Pa×s	434.96	Joback Method
dvisc	0.0004835	Pa×s	477.68	Joback Method
dvisc	0.0003896	Pa×s	520.41	Joback Method
dvisc	0.0003244	Pa×s	563.13	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=C35365527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid 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