

Cyclopropane, 1,1-dichloro-2-hexyl-3-phenyl

Inchi:	InChI=1S/C15H20Cl2/c1-2-3-4-8-11-13-14(15(13,16)17)12-9-6-5-7-10-12/h5-7,9-10,13-1
InchiKey:	OUVKISAYBHYIDE-UHFFFAOYSA-N
Formula:	C15H20Cl2
SMILES:	CCCCCCC1C(c2ccccc2)C1(Cl)Cl
Mol. weight [g/mol]:	271.23

Physical Properties

Property code	Value	Unit	Source
gf	203.81	kJ/mol	Joback Method
hf	-100.52	kJ/mol	Joback Method
hfus	31.02	kJ/mol	Joback Method
hvap	58.17	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.544		Crippen Method
mcvol	212.070	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1783.00		NIST Webbook
ripol	2321.00		NIST Webbook
ripol	2321.00		NIST Webbook
tb	641.78	K	Joback Method
tc	862.09	K	Joback Method
tf	378.43	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.48	J/molxK	641.78	Joback Method
cpg	561.33	J/molxK	678.50	Joback Method
cpg	578.15	J/molxK	715.22	Joback Method
cpg	594.10	J/molxK	751.94	Joback Method
cpg	609.34	J/molxK	788.65	Joback Method
cpg	624.04	J/molxK	825.37	Joback Method

Sources

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=R122097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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