

cis-1,2-Diethylcyclopropane

Inchi:	InChI=1S/C7H14/c1-3-6-5-7(6)4-2/h6-7H,3-5H2,1-2H3/t6-,7+
InchiKey:	AKOVCHSGJHQHEH-KNVOCYPGSA-N
Formula:	C7H14
SMILES:	CCC1CC1CC
Mol. weight [g/mol]:	98.19
CAS:	71032-67-2

Physical Properties

Property code	Value	Unit	Source
chl	-4675.00 ± 1.00	kJ/mol	NIST Webbook
gf	61.10	kJ/mol	Joback Method
hf	-44.60 ± 1.60	kJ/mol	NIST Webbook
hfl	-80.00 ± 1.40	kJ/mol	NIST Webbook
hfus	13.09	kJ/mol	Joback Method
hvap	35.40 ± 0.80	kJ/mol	NIST Webbook
hvap	35.40	kJ/mol	NIST Webbook
log10ws	-2.16		Crippen Method
logp	2.442		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	695.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	694.80		NIST Webbook
tb	366.65 ± 2.00	K	NIST Webbook
tc	539.10	K	Joback Method
tf	182.35	K	Joback Method
vc	0.384	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.61	J/mol×K	361.63	Joback Method
cpg	191.26	J/mol×K	391.21	Joback Method
cpg	204.28	J/mol×K	420.79	Joback Method

cpg	216.71	J/mol×K	450.36	Joback Method
cpg	228.57	J/mol×K	479.94	Joback Method
cpg	239.87	J/mol×K	509.52	Joback Method
cpg	250.64	J/mol×K	539.10	Joback Method
dvisc	0.0004919	Paxs	182.35	Joback Method
dvisc	0.0004196	Paxs	212.23	Joback Method
dvisc	0.0003722	Paxs	242.11	Joback Method
dvisc	0.0003390	Paxs	271.99	Joback Method
dvisc	0.0003145	Paxs	301.87	Joback Method
dvisc	0.0002957	Paxs	331.75	Joback Method
dvisc	0.0002809	Paxs	361.63	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=C71032672&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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