

cis-1,2-Divinylcyclobutane

Other names:	cis-1,2-Diethenyl-cyclobutane Cyclobutane, cis-1,2-diethenyl- Cyclobutane, 1,2-diethenyl-, cis- Cyclobutane, (Z)-1,2-diethenyl (Z)-1,2-Divinylcyclobutane
Inchi:	InChI=1S/C8H12/c1-3-7-5-6-8(7)4-2/h3-4,7-8H,1-2,5-6H2/t7-,8+
InchiKey:	UHHCYAAVGADGGP-OCAPTIKFSAN
Formula:	C8H12
SMILES:	C=CC1CCC1C=C
Mol. weight [g/mol]:	108.18
CAS:	16177-46-1

Physical Properties

Property code	Value	Unit	Source
chl	-4987.30	kJ/mol	NIST Webbook
gf	233.10	kJ/mol	Joback Method
hf	188.00 ± 5.50	kJ/mol	NIST Webbook
hfus	11.02	kJ/mol	Joback Method
hvap	42.26	kJ/mol	NIST Webbook
ie	9.22	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	2.385		Crippen Method
mvol	104.120	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	382.14	K	Joback Method
tc	574.70	K	Joback Method
tf	186.58	K	Joback Method
vc	0.394	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.55	J/mol×K	382.14	Joback Method
cpg	200.19	J/mol×K	414.23	Joback Method

cpg	214.06	J/molxK	446.33	Joback Method
cpg	227.19	J/molxK	478.42	Joback Method
cpg	239.60	J/molxK	510.51	Joback Method
cpg	251.33	J/molxK	542.61	Joback Method
cpg	262.41	J/molxK	574.70	Joback Method
dvisc	0.0008087	Paxs	186.58	Joback Method
dvisc	0.0005958	Paxs	219.17	Joback Method
dvisc	0.0004751	Paxs	251.77	Joback Method
dvisc	0.0003990	Paxs	284.36	Joback Method
dvisc	0.0003474	Paxs	316.95	Joback Method
dvisc	0.0003104	Paxs	349.55	Joback Method
dvisc	0.0002827	Paxs	382.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	311.20	K	5.10	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16177461&Units=SI>

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>

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

ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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