

Cyclobutane, 1,2-diethenyl-, trans-

Other names:	(E)-1,2-Divinylcyclobutane Cyclobutane, 1,2-divinyl-, trans- Cyclobutane,trans-1,2-diethenyl- trans-1,2-Diethenyl-cyclobutane trans-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-/m1/s1
InchiKey:	UHHCYAAVGADGGP-HTQZYQBOSA-N
Formula:	C8H12
SMILES:	C=CC1CCC1C=C
Mol. weight [g/mol]:	108.18
CAS:	6553-48-6

Physical Properties

Property code	Value	Unit	Source
chl	-4964.30	kJ/mol	NIST Webbook
gf	233.10	kJ/mol	Joback Method
hf	177.00	kJ/mol	NIST Webbook
hfus	11.02	kJ/mol	Joback Method
hvap	42.26	kJ/mol	NIST Webbook
hvap	38.90 ± 0.50	kJ/mol	NIST Webbook
hvap	42.30	kJ/mol	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	2.385		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	385.70	K	NIST Webbook
tc	574.70	K	Joback Method
tf	186.58	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	251.33	J/mol×K	542.61	Joback Method
cpg	262.41	J/mol×K	574.70	Joback Method
cpg	185.55	J/mol×K	382.14	Joback Method
cpg	200.19	J/mol×K	414.23	Joback Method
cpg	214.06	J/mol×K	446.33	Joback Method
cpg	227.19	J/mol×K	478.42	Joback Method
cpg	239.60	J/mol×K	510.51	Joback Method
dvisc	0.0002827	Pa×s	382.14	Joback Method
dvisc	0.0003104	Pa×s	349.55	Joback Method
dvisc	0.0008087	Pa×s	186.58	Joback Method
dvisc	0.0005958	Pa×s	219.17	Joback Method
dvisc	0.0004751	Pa×s	251.77	Joback Method
dvisc	0.0003990	Pa×s	284.36	Joback Method
dvisc	0.0003474	Pa×s	316.95	Joback Method
hvapt	39.00 ± 0.50	kJ/mol	367.00	NIST Webbook
hvapt	39.10	kJ/mol	367.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.14746e+01
Coeff. B	-2.81793e+03
Temperature range (K), min.	251.89
Temperature range (K), max.	457.23

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6553486&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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