cis-1,3-Diethenylcyclobutane

Inchi: InChI=1S/C8H12/c1-3-7-5-8(4-2)6-7/h3-4,7-8H,1-2,5-6H2/t7-,8+
InchiKey: AATSALLMQGUKIE-OCAPTIKFSA-N
Formula: C8H12
SMILES: C=CC1CC(C=C)C1
Mol. weight [g/mol]: 108.18
CAS: 77614-53-0

Physical Properties

Property code	Value	Unit	Source
gf	233.10	kJ/mol	Joback Method
hf	88.71	kJ/mol	Joback Method
hfus	11.02	kJ/mol	Joback Method
hvap	31.84	kJ/mol	Joback Method
ie	9.38	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	382.14	K	Joback Method
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
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
cpg	251.33	J/mol×K	542.61	Joback Method
cpg	262.41	J/mol×K	574.70	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
dvisc	0.0003104	Pa×s	349.55	Joback Method
dvisc	0.0002827	Pa×s	382.14	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=C77614530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume