trans-1,2-Diethyl-cyclopropane

Inchi: InChI=1S/C7H14/c1-3-6-5-7(6)4-2/h6-7H,3-5H2,1-2H3/t6-,7-/m0/s1
InchiKey: AKOVCHSGJHQHEH-BQBZGAKWSA-N
Formula: C7H14
SMILES: CCC1CC1CC
Mol. weight [g/mol]: 98.19
CAS: 71032-66-1

Physical Properties

Property code	Value	Unit	Source
chl	-4672.10 ± 1.50	kJ/mol	NIST Webbook
gf	61.10	kJ/mol	Joback Method
hf	-49.10 ± 1.80	kJ/mol	NIST Webbook
hfl	-83.40 ± 1.60	kJ/mol	NIST Webbook
hfus	13.09	kJ/mol	Joback Method
hvap	34.30 ± 0.84	kJ/mol	NIST Webbook
hvap	34.30	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	663.00		NIST Webbook
rinpol	662.80		NIST Webbook
rinpol	663.00		NIST Webbook
tb	359.65 ± 2.00	K	NIST Webbook
tc	539.10	K	Joback Method
tf	182.35	K	Joback Method
vc	0.384	m3/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	Pa×s	182.35	Joback Method
dvisc	0.0004196	Pa×s	212.23	Joback Method
dvisc	0.0003722	Pa×s	242.11	Joback Method
dvisc	0.0003390	Pa×s	271.99	Joback Method
dvisc	0.0003145	Pa×s	301.87	Joback Method
dvisc	0.0002957	Pa×s	331.75	Joback Method
dvisc	0.0002809	Pa×s	361.63	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71032661&Units=SI

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