trans-1-Ethyl-2-methylcyclopropane

Other names: 1-Methyl-trans-2-ethyl-cyclopropane
cyclopropane, 1-ethyl-2-methyl-, trans-
Inchi: InChI=1S/C6H12/c1-3-6-4-5(6)2/h5-6H,3-4H2,1-2H3
InchiKey: SAHWBARCQUAFSM-UHFFFAOYSA-N
Formula: C6H12
SMILES: CCC1CC1C
Mol. weight [g/mol]: 84.16
CAS: 19781-69-2

Physical Properties

Property code	Value	Unit	Source
gf	52.68	kJ/mol	Joback Method
hf	-114.71	kJ/mol	Joback Method
hfus	10.50	kJ/mol	Joback Method
hvap	28.55	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	2.052		Crippen Method
mcvol	84.540	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	568.00		NIST Webbook
rinpol	568.00		NIST Webbook
tb	332.10 ± 0.70	K	NIST Webbook
tb	331.81 ± 0.30	K	NIST Webbook
tc	516.38	K	Joback Method
tf	171.08	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	141.13	J/mol×K	338.75	Joback Method
cpg	153.47	J/mol×K	368.36	Joback Method
cpg	165.26	J/mol×K	397.96	Joback Method
cpg	176.49	J/mol×K	427.57	Joback Method

cpg	187.20	J/mol×K	457.17	Joback Method
cpg	197.41	J/mol×K	486.78	Joback Method
cpg	207.14	J/mol×K	516.38	Joback Method
dvisc	0.0003196	Pa×s	171.08	Joback Method
dvisc	0.0002916	Pa×s	199.02	Joback Method
dvisc	0.0002721	Pa×s	226.97	Joback Method
dvisc	0.0002578	Pa×s	254.91	Joback Method
dvisc	0.0002468	Pa×s	282.86	Joback Method
dvisc	0.0002382	Pa×s	310.81	Joback Method
dvisc	0.0002312	Pa×s	338.75	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=C19781692&Units=SI

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
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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