Cyclopropane, 1-ethyl-1-methyl-

Other names: 1-Ethyl-1-methylcyclopropane
Inchi: InChI=1S/C6H12/c1-3-6(2)4-5-6/h3-5H2,1-2H3
InchiKey: CXYUCHDVLWUDNS-UHFFFAOYSA-N
Formula: C6H12
SMILES: CCC1(C)CC1
Mol. weight [g/mol]: 84.16
CAS: 53778-43-1

Physical Properties

Property code	Value	Unit	Source
gf	54.90	kJ/mol	Joback Method
hf	-79.13	kJ/mol	Joback Method
hfus	3.13	kJ/mol	Joback Method
hvap	27.71	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.196		Crippen Method
mcvol	84.540	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
rinpol	567.00		NIST Webbook
rinpol	567.00		NIST Webbook
rinpol	567.00		NIST Webbook
rinpol	567.00		NIST Webbook
tb	329.92 ± 0.30	K	NIST Webbook
tb	329.90 ± 1.00	K	NIST Webbook
tb	329.94 ± 0.20	K	NIST Webbook
tc	530.57	K	Joback Method
tf	142.94 ± 0.20	K	NIST Webbook
tf	142.92 ± 0.20	K	NIST Webbook
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.50	J/mol×K	343.66	Joback Method

cpg	154.07	J/mol×K	374.81	Joback Method
cpg	166.59	J/mol×K	405.96	Joback Method
cpg	178.14	J/mol×K	437.11	Joback Method
cpg	188.81	J/mol×K	468.27	Joback Method
cpg	198.68	J/mol×K	499.42	Joback Method
cpg	207.83	J/mol×K	530.57	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=C53778431&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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