1,1-Dimethyl-2-ethyl-cyclopropane

Inchi: InChI=1S/C7H14/c1-4-6-5-7(6,2)3/h6H,4-5H2,1-3H3
InchiKey: UDCRTPSZNQOKRO-UHFFFAOYSA-N
Formula: C7H14
SMILES: CCC1CC1(C)C
Mol. weight [g/mol]: 98.19
CAS: 41845-47-0

Physical Properties

Property code	Value	Unit	Source
chl	-4665.20 ± 0.80	kJ/mol	NIST Webbook
gf	55.61	kJ/mol	Joback Method
hf	-120.11	kJ/mol	Joback Method
hfl	-90.40 ± 0.92	kJ/mol	NIST Webbook
hfus	6.79	kJ/mol	Joback Method
hvap	29.63	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.442		Crippen Method
mcvol	98.630	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	632.80		NIST Webbook
rinpol	632.80		NIST Webbook
tb	361.87	K	Joback Method
tc	547.57	K	Joback Method
tf	206.25	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.75	J/mol×K	361.87	Joback Method
cpg	192.55	J/mol×K	392.82	Joback Method
cpg	206.32	J/mol×K	423.77	Joback Method
cpg	219.14	J/mol×K	454.72	Joback Method
cpg	231.10	J/mol×K	485.67	Joback Method

cpg	242.27	J/mol×K	516.62	Joback Method
cpg	252.73	J/mol×K	547.57	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=C41845470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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