1,1-Dimethyl-2-propyl-cyclopropane

Inchi: InChI=1S/C8H16/c1-4-5-7-6-8(7,2)3/h7H,4-6H2,1-3H3
InchiKey: NWQWWOHNBLAJQT-UHFFFAOYSA-N
Formula: C8H16
SMILES: CCCC1CC1(C)C
Mol. weight [g/mol]: 112.21
CAS: 41845-48-1

Physical Properties

Property code	Value	Unit	Source
chl	-5319.00 ± 2.00	kJ/mol	NIST Webbook
gf	64.03	kJ/mol	Joback Method
hf	-140.75	kJ/mol	Joback Method
hfl	-116.40	kJ/mol	NIST Webbook
hfus	9.38	kJ/mol	Joback Method
hvap	31.86	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	727.40		NIST Webbook
tb	378.65 ± 0.40	K	NIST Webbook
tc	569.64	K	Joback Method
tf	217.52	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.06	J/mol×K	384.75	Joback Method
cpg	232.79	J/mol×K	415.56	Joback Method
cpg	247.49	J/mol×K	446.38	Joback Method
cpg	261.23	J/mol×K	477.19	Joback Method
cpg	274.10	J/mol×K	508.01	Joback Method
cpg	286.18	J/mol×K	538.82	Joback Method

cpg	297.55	J/mol×K	569.64	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=C41845481&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

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