

Cyclopropane,1,2-dimethyl-3-(2-methyl-1-propeny

Inchi:	InChI=1S/C9H14/c1-6(2)5-9-7(3)8(9)4/h7-8H,1-4H3/t7-,8+
InchiKey:	VAZXLGQWHLNHOI-OCAPTIKFSA-N
Formula:	C9H14
SMILES:	CC(C)=C=C1C(C)C1C
Mol. weight [g/mol]:	122.21
CAS:	37817-36-0

Physical Properties

Property code	Value	Unit	Source
gf	243.13	kJ/mol	Joback Method
hf	52.39	kJ/mol	Joback Method
hfus	19.42	kJ/mol	Joback Method
hvap	36.53	kJ/mol	Joback Method
ie	7.76	eV	NIST Webbook
log10ws	-2.73		Crippen Method
logp	2.764		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
tb	417.18	K	Joback Method
tc	615.67	K	Joback Method
tf	207.80	K	Joback Method
vc	0.460	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.27	J/molxK	417.18	Joback Method
cpg	249.46	J/molxK	450.26	Joback Method
cpg	262.99	J/molxK	483.34	Joback Method
cpg	275.88	J/molxK	516.43	Joback Method
cpg	288.17	J/molxK	549.51	Joback Method
cpg	299.86	J/molxK	582.59	Joback Method
cpg	310.99	J/molxK	615.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37817360&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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