

Cyclopropane, 1,1-dimethyl-2-nonyl-

Inchi:	InChI=1S/C14H28/c1-4-5-6-7-8-9-10-11-13-12-14(13,2)3/h13H,4-12H2,1-3H3
InchiKey:	PMTRHHGOQMLDQB-UHFFFAOYSA-N
Formula:	C14H28
SMILES:	CCCCCCCCC1CC1(C)C
Mol. weight [g/mol]:	196.37
CAS:	41977-38-2

Physical Properties

Property code	Value	Unit	Source
gf	114.55	kJ/mol	Joback Method
hf	-264.59	kJ/mol	Joback Method
hfus	24.92	kJ/mol	Joback Method
hvap	45.21	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	5.173		Crippen Method
mcvol	197.260	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
tb	522.03	K	Joback Method
tc	698.04	K	Joback Method
tf	285.14	K	Joback Method
vc	0.773	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.01	J/mol×K	522.03	Joback Method
cpg	512.45	J/mol×K	551.37	Joback Method
cpg	530.93	J/mol×K	580.70	Joback Method
cpg	548.50	J/mol×K	610.04	Joback Method
cpg	565.26	J/mol×K	639.37	Joback Method
cpg	581.27	J/mol×K	668.71	Joback Method
cpg	596.63	J/mol×K	698.04	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=C41977382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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