

Veloutone

Inchi:	InChI=1S/C13H24O/c1-5-6-7-8-13(4)10-9-12(2,3)11(13)14/h5-10H2,1-4H3
InchiKey:	PUKWIVZFEZVAT-UHFFFAOYSA-N
Formula:	C13H24O
SMILES:	CCCCC1(C)CCC(C)(C)C1=O
Mol. weight [g/mol]:	196.33

Physical Properties

Property code	Value	Unit	Source
gf	-46.15	kJ/mol	Joback Method
hf	-378.73	kJ/mol	Joback Method
hfus	11.35	kJ/mol	Joback Method
hvap	46.42	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.962		Crippen Method
mcvol	184.740	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpola	1306.00		NIST Webbook
rinpola	1306.00		NIST Webbook
tb	575.75	K	Joback Method
tc	788.11	K	Joback Method
tf	358.95	K	Joback Method
vc	0.707	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.15	J/molxK	575.75	Joback Method
cpg	505.06	J/molxK	611.14	Joback Method
cpg	523.94	J/molxK	646.54	Joback Method
cpg	541.98	J/molxK	681.93	Joback Method
cpg	559.33	J/molxK	717.32	Joback Method
cpg	576.17	J/molxK	752.72	Joback Method
cpg	592.67	J/molxK	788.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R607048&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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