

mustakone

Inchi:	InChI=1S/C14H20O/c1-8(2)9-6-7-14(3)10-4-5-11(15)13(14)12(9)10/h4-5,8-10,12-13H,6-7
InchiKey:	GZLLVGOKTRVUIU-BIMVQAMKSA-N
Formula:	C14H20O
SMILES:	CC(C)C1CCC2(C)C3C=CC(=O)C2C13
Mol. weight [g/mol]:	204.31

Physical Properties

Property code	Value	Unit	Source
gf	121.17	kJ/mol	Joback Method
hf	-230.69	kJ/mol	Joback Method
hfus	17.37	kJ/mol	Joback Method
hvap	49.05	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.060		Crippen Method
mcvol	172.810	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinqol	1653.00		NIST Webbook
tb	601.65	K	Joback Method
tc	831.96	K	Joback Method
tf	367.24	K	Joback Method
vc	0.665	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.88	J/mol×K	601.65	Joback Method
cpg	512.09	J/mol×K	640.04	Joback Method
cpg	531.96	J/mol×K	678.42	Joback Method
cpg	550.69	J/mol×K	716.81	Joback Method
cpg	568.46	J/mol×K	755.19	Joback Method
cpg	585.45	J/mol×K	793.58	Joback Method
cpg	601.87	J/mol×K	831.96	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=R334295&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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