dihydromethylionone

Inchi: InChI=1S/C14H24O/c1-10-7-6-8-14(4,5)13(10)9-11(2)12(3)15/h7,11,13H,6,8-9H2,1-5H3
InchiKey: SYLQLBRNBHRVCR-UHFFFAOYSA-N
Formula: C14H24O
SMILES: CC(=O)C(C)CC1C(C)=CCCC1(C)C
Mol. weight [g/mol]: 208.34

Physical Properties

Property code	Value	Unit	Source
gf	-32.78	kJ/mol	Joback Method
hf	-354.62	kJ/mol	Joback Method
hfus	17.53	kJ/mol	Joback Method
hvap	53.04	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.984		Crippen Method
mcvol	194.530	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
ripol	1967.00		NIST Webbook
ripol	1967.00		NIST Webbook
tb	592.41	K	Joback Method
tc	802.16	K	Joback Method
tf	322.79	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.23	J/mol×K	592.41	Joback Method
cpg	529.18	J/mol×K	627.37	Joback Method
cpg	548.06	J/mol×K	662.33	Joback Method
cpg	565.97	J/mol×K	697.29	Joback Method
cpg	583.01	J/mol×K	732.24	Joback Method
cpg	599.29	J/mol×K	767.20	Joback Method
cpg	614.91	J/mol×K	802.16	Joback Method

Sources

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=R315630&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume