11,12-Dihydrochiloscyphone

Inchi: InChI=1S/C15H24O/c1-10(2)14(16)13-9-8-12-7-5-6-11(3)15(12,13)4/h7,10-11,13H,5-6,8-
InchiKey: DVAATBRDCVSPRO-NJZAAPMLSA-N
Formula: C15H24O
SMILES: CC(C)C(=O)C1CCC2=CCCC(C)C21C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	36.39	kJ/mol	Joback Method
hf	-302.46	kJ/mol	Joback Method
hfus	18.26	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.984		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook
tb	622.03	K	Joback Method
tc	842.78	K	Joback Method
tf	352.00	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.52	J/mol×K	622.03	Joback Method
cpg	569.66	J/mol×K	658.82	Joback Method
cpg	589.58	J/mol×K	695.61	Joback Method
cpg	608.41	J/mol×K	732.40	Joback Method
cpg	626.31	J/mol×K	769.20	Joback Method
cpg	643.45	J/mol×K	805.99	Joback Method
cpg	659.96	J/mol×K	842.78	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=R281577&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
mcvol:	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