

Dihydrochiloscypholone

Inchi:	InChI=1S/C15H26O2/c1-10(2)13(16)12-7-9-15(17)8-5-6-11(3)14(12,15)4/h10-12,17H,5-9
InchiKey:	HUQLDUXYHVFPRA-MYZSUADSSA-N
Formula:	C15H26O2
SMILES:	CC(C)C(=O)C1CCC2(O)CCCC(C)C12C
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-133.96	kJ/mol	Joback Method
hf	-506.10	kJ/mol	Joback Method
hfus	16.29	kJ/mol	Joback Method
hvap	69.44	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.179		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	705.64	K	Joback Method
tc	915.62	K	Joback Method
tf	419.20	K	Joback Method
vc	0.778	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.79	J/mol×K	705.64	Joback Method
cpg	658.75	J/mol×K	740.64	Joback Method
cpg	677.10	J/mol×K	775.63	Joback Method
cpg	695.05	J/mol×K	810.63	Joback Method
cpg	712.81	J/mol×K	845.63	Joback Method
cpg	730.59	J/mol×K	880.63	Joback Method
cpg	748.59	J/mol×K	915.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R281631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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