7,10-Anhydro-11,12-dihydrochiloscypholone

Inchi: InChI=1S/C15H24O2/c1-10(2)13(16)12-7-9-15(17)8-5-6-11(3)14(12,15)4/h7,10-11,17H,5
InchiKey: ANEQSEHKTRCMOT-TUKIKUTGSA-N
Formula: C15H24O2
SMILES: CC(C)C(=O)C1=CCC2(O)CCCC(C)C12C
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-105.92	kJ/mol	Joback Method
hf	-439.45	kJ/mol	Joback Method
hfus	16.05	kJ/mol	Joback Method
hvap	70.71	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.099		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1452.00		NIST Webbook
rinpol	1452.00		NIST Webbook
tb	714.45	K	Joback Method
tc	926.90	K	Joback Method
tf	436.72	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.35	J/mol×K	714.45	Joback Method
cpg	629.90	J/mol×K	749.86	Joback Method
cpg	646.98	J/mol×K	785.27	Joback Method
cpg	663.81	J/mol×K	820.67	Joback Method
cpg	680.62	J/mol×K	856.08	Joback Method
cpg	697.61	J/mol×K	891.49	Joback Method
cpg	715.02	J/mol×K	926.90	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=R281582&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume