

Uvidin A

Inchi:	InChI=1S/C15H24O3/c1-13(2)6-5-7-14(3)9(8-16)15(4)12(18-15)10(17)11(13)14/h9,11-12
InchiKey:	AHPUPUJYVYUVKA-BRIGZHOFSA-N
Formula:	C15H24O3
SMILES:	CC1(C)CCCC2(C)C1C(=O)C1OC1(C)C2CO
Mol. weight [g/mol]:	252.35

Physical Properties

Property code	Value	Unit	Source
gf	-151.66	kJ/mol	Joback Method
hf	-584.08	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	70.12	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.168		Crippen Method
mcvol	202.940	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	2081.00		NIST Webbook
rinpol	2081.00		NIST Webbook
tb	745.02	K	Joback Method
tc	967.21	K	Joback Method
tf	520.18	K	Joback Method
vc	0.768	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.44	J/mol×K	745.02	Joback Method
cpg	686.25	J/mol×K	782.05	Joback Method
cpg	706.13	J/mol×K	819.08	Joback Method
cpg	726.40	J/mol×K	856.11	Joback Method
cpg	747.42	J/mol×K	893.14	Joback Method
cpg	769.50	J/mol×K	930.18	Joback Method
cpg	793.00	J/mol×K	967.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R435620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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