Cryptofauronol

Inchi: InChI=1S/C15H26O2/c1-10(2)11-8-14(4)13(3)6-5-7-15(14,16)17-12(11)9-13/h10-12,16H
InchiKey: UTNQUNGFEKWBQT-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: CC(C)C1CC2(C)C3(C)CCCC2(O)OC1C3
Mol. weight [g/mol]: 238.37
CAS: 2212-90-0

Physical Properties

Property code	Value	Unit	Source
gf	-23.80	kJ/mol	Joback Method
hf	-431.32	kJ/mol	Joback Method
hfus	16.60	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.336		Crippen Method
mcvol	201.370	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1644.00		NIST Webbook
tb	681.43	K	Joback Method
tc	896.88	K	Joback Method
tf	441.20	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.32	J/mol×K	681.43	Joback Method
cpg	647.61	J/mol×K	717.34	Joback Method
cpg	666.42	J/mol×K	753.25	Joback Method
cpg	685.08	J/mol×K	789.15	Joback Method
cpg	703.94	J/mol×K	825.06	Joback Method
cpg	723.34	J/mol×K	860.97	Joback Method
cpg	743.64	J/mol×K	896.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2212900&Units=SI

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