Cryptofauronyl acetate

Inchi: InChI=1S/C16H26O3/c1-9(2)11-7-12-15-13(18-10(3)17)5-6-16(12,4)8-14(11)19-15/h9,11
InchiKey: IHEPBMIPFUVAAE-IXWGYMPFSA-N
Formula: C16H26O3
SMILES: CC(=O)OC1CCC2(C)CC3OC1C2CC3C(C)C
Mol. weight [g/mol]: 266.38

Physical Properties

Property code	Value	Unit	Source
gf	-109.21	kJ/mol	Joback Method
hf	-595.35	kJ/mol	Joback Method
hfus	31.56	kJ/mol	Joback Method
hvap	62.49	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.168		Crippen Method
mcvol	217.030	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	683.27	K	Joback Method
tc	899.92	K	Joback Method
tf	411.77	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.97	J/mol×K	683.27	Joback Method
cpg	699.76	J/mol×K	719.38	Joback Method
cpg	720.42	J/mol×K	755.49	Joback Method
cpg	740.09	J/mol×K	791.60	Joback Method
cpg	758.95	J/mol×K	827.71	Joback Method
cpg	777.13	J/mol×K	863.81	Joback Method
cpg	794.80	J/mol×K	899.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224727&Units=SI
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

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