killarniensolide, acetylated

Inchi: InChI=1S/C20H20O7/c1-11(21)26-15-10-18(25-4)17(24-3)9-12(15)8-16-13-6-5-7-14(23-2
InchiKey: ABGLNBXETPHZGG-UHFFFAOYSA-N
Formula: C20H20O7
SMILES: COc1cc(CC2OC(=O)c3c(OC)cccc32)c(OC(C)=O)cc1OC
Mol. weight [g/mol]: 372.37

Physical Properties

Property code	Value	Unit	Source
gf	-402.69	kJ/mol	Joback Method
hf	-878.78	kJ/mol	Joback Method
hfus	45.67	kJ/mol	Joback Method
hvap	93.03	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.092		Crippen Method
mcvol	266.770	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	2806.00		NIST Webbook
rinpol	2806.00		NIST Webbook
tb	980.32	K	Joback Method
tc	1218.40	K	Joback Method
tf	682.18	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.70	J/mol×K	980.32	Joback Method
cpg	865.53	J/mol×K	1020.00	Joback Method
cpg	874.52	J/mol×K	1059.68	Joback Method
cpg	881.61	J/mol×K	1099.36	Joback Method
cpg	886.78	J/mol×K	1139.04	Joback Method
cpg	889.98	J/mol×K	1178.72	Joback Method
cpg	891.18	J/mol×K	1218.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R273957&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