killarniensolide

Inchi: InChI=1S/C18H18O6/c1-21-13-6-4-5-11-14(24-18(20)17(11)13)7-10-8-15(22-2)16(23-3)9
InchiKey: GERFPYQYRDPXMX-UHFFFAOYSA-N
Formula: C18H18O6
SMILES: COc1cc(O)c(CC2OC(=O)c3c(OC)cccc32)cc1OC
Mol. weight [g/mol]: 330.33
CAS: 230291-26-6

Physical Properties

Property code	Value	Unit	Source
gf	-330.60	kJ/mol	Joback Method
hf	-758.54	kJ/mol	Joback Method
hfus	43.87	kJ/mol	Joback Method
hvap	91.78	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.872		Crippen Method
mcvol	237.020	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	2775.00		NIST Webbook
rinpol	2775.00		NIST Webbook
tb	933.91	K	Joback Method
tc	1178.20	K	Joback Method
tf	686.68	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.14	J/mol×K	933.91	Joback Method
cpg	767.38	J/mol×K	974.63	Joback Method
cpg	779.50	J/mol×K	1015.34	Joback Method
cpg	790.52	J/mol×K	1056.06	Joback Method
cpg	800.50	J/mol×K	1096.77	Joback Method
cpg	809.47	J/mol×K	1137.49	Joback Method
cpg	817.47	J/mol×K	1178.20	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=C230291266&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