Ferutinin

Inchi: InChI=1S/C22H30O4/c1-14(2)22(25)12-11-21(4)10-9-15(3)13-18(19(21)22)26-20(24)16-
InchiKey: CYSHNJQMYORNJI-WAGURGNTSA-N
Formula: C22H30O4
SMILES: CC1=CCC2(C)CCC(O)(C(C)C)C2C(OC(=O)c2ccc(O)cc2)C1
Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-214.00	kJ/mol	Joback Method
hf	-683.43	kJ/mol	Joback Method
hfus	34.16	kJ/mol	Joback Method
hvap	103.85	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.461		Crippen Method
mcvol	290.240	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	2684.00		NIST Webbook
tb	1003.93	K	Joback Method
tc	1244.36	K	Joback Method
tf	668.22	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1047.81	J/mol×K	1003.93	Joback Method
cpg	1075.31	J/mol×K	1044.00	Joback Method
cpg	1104.38	J/mol×K	1084.07	Joback Method
cpg	1135.40	J/mol×K	1124.14	Joback Method
cpg	1168.72	J/mol×K	1164.21	Joback Method
cpg	1204.71	J/mol×K	1204.29	Joback Method
cpg	1243.75	J/mol×K	1244.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R200276&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

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