medinoterb acetate

Inchi: InChI=1S/C13H16N2O6/c1-7-10(14(17)18)6-9(13(3,4)5)12(21-8(2)16)11(7)15(19)20/h6H
InchiKey: LWULXYSYLOIDQY-UHFFFAOYSA-N
Formula: C13H16N2O6
SMILES: CC(=O)Oc1c(C(C)(C)C)cc([N+](=O)[O-])c(C)c1[N+](=O)[O-]
Mol. weight [g/mol]: 296.28

Physical Properties

Property code	Value	Unit	Source
gf	-27.51	kJ/mol	Joback Method
hf	-396.07	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	90.50	kJ/mol	Joback Method
log10ws	-4.47		Aqueous Solubility Prediction Method
logp	3.034		Crippen Method
mcvol	212.550	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
tb	920.18	K	Joback Method
tc	1174.94	K	Joback Method
tf	359.65	K	Aqueous Solubility Prediction Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.61	J/mol×K	920.18	Joback Method
cpg	652.29	J/mol×K	962.64	Joback Method
cpg	661.86	J/mol×K	1005.10	Joback Method
cpg	670.38	J/mol×K	1047.56	Joback Method
cpg	677.90	J/mol×K	1090.02	Joback Method
cpg	684.47	J/mol×K	1132.48	Joback Method
cpg	690.15	J/mol×K	1174.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume