aceclofenac

Inchi: InChI=1S/C16H13Cl2NO4/c17-11-5-3-6-12(18)16(11)19-13-7-2-1-4-10(13)8-15(22)23-9-
InchiKey: MNIPYSSQXLZQLJ-UHFFFAOYSA-N
Formula: C16H13Cl2NO4
SMILES: O=C(O)COC(=O)Cc1ccccc1Nc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 354.19

Physical Properties

Property code	Value	Unit	Source
gf	-154.36	kJ/mol	Joback Method
hf	-422.54	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	105.53	kJ/mol	Joback Method
log10ws	-2.54		Aqueous Solubility Prediction Method
logp	3.907		Crippen Method
mcvol	238.120	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
tb	981.15	K	Joback Method
tc	1215.61	K	Joback Method
tf	655.89	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.44	J/mol×K	981.15	Joback Method
cpg	671.09	J/mol×K	1020.23	Joback Method
cpg	677.81	J/mol×K	1059.30	Joback Method
cpg	683.62	J/mol×K	1098.38	Joback Method
cpg	688.57	J/mol×K	1137.46	Joback Method
cpg	692.71	J/mol×K	1176.54	Joback Method
cpg	696.07	J/mol×K	1215.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

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