Meclofenamic Acid

Inchi: InChI=1S/C14H11Cl2NO2/c1-8-6-7-10(15)13(12(8)16)17-11-5-3-2-4-9(11)14(18)19/h2-7
InchiKey: SBDNJUWAMKYJOX-UHFFFAOYSA-N
Formula: C14H11Cl2NO2
SMILES: Cc1ccc(Cl)c(Nc2ccccc2C(=O)O)c1Cl
Mol. weight [g/mol]: 296.15
CAS: 644-62-2

Physical Properties

Property code	Value	Unit	Source
gf	53.09	kJ/mol	Joback Method
hf	-147.93	kJ/mol	Joback Method
hfus	37.72	kJ/mol	Joback Method
hvap	92.59	kJ/mol	Joback Method
log10ws	-6.27		Aqueous Solubility Prediction Method
logp	4.744		Crippen Method
mcvol	202.500	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook
tb	864.08	K	Joback Method
tc	1097.06	K	Joback Method
tf	573.71	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.13	J/mol×K	864.08	Joback Method
cpg	534.20	J/mol×K	902.91	Joback Method
cpg	542.48	J/mol×K	941.74	Joback Method
cpg	550.01	J/mol×K	980.57	Joback Method
cpg	556.84	J/mol×K	1019.40	Joback Method

cpg	563.01	J/mol×K	1058.23	Joback Method
cpg	568.57	J/mol×K	1097.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C644622&Units=SI
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/AqueousDataset003.xlsx/351830174/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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume