Diclofenac

Other names:	2-[(2,6-Dichlorophenyl)amino]benzeneacetic acid
	2-[(2,6-Dichlorophenyl)amino]benzoic acid (diclofenac acid)
	Acetic acid, (o-(2,6-dichloroanilino)phenyl)-
	Benzeneacetic acid, 2-[(2,6-dichlorophenyl)amino]-
	Dichlofenac
	Diclofenac acid
Inchi:	InChI=1S/C14H11Cl2NO2/c15-10-5-3-6-11(16)14(10)17-12-7-2-1-4-9(12)8-13(18)19/h1-
InchiKey:	DCOPUUMXTXDBNB-UHFFFAOYSA-N
Formula:	C14H11Cl2NO2
SMILES:	O=C(O)Cc1ccccc1Nc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	296.15
CAS:	15307-86-5

Physical Properties

Property code	Value	Unit	Source
gf	62.72	kJ/mol	Joback Method
hf	-136.46	kJ/mol	Joback Method
hfus	38.11	kJ/mol	Joback Method
hsub	115.60 ± 1.30	kJ/mol	NIST Webbook
hvap	91.93	kJ/mol	Joback Method
log10ws	-5.10		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-5.46		Aqueous Solubility Prediction Method
logp	4.364		Crippen Method
mcvol	202.500	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
tb	859.10	K	Joback Method
tc	1091.35	K	Joback Method
tf	436.53	K	Aqueous Solubility Prediction Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.01	J/mol×K	859.10	Joback Method
cpg	536.14	J/mol×K	897.81	Joback Method
cpg	544.47	J/mol×K	936.52	Joback Method
cpg	552.06	J/mol×K	975.23	Joback Method
cpg	558.96	J/mol×K	1013.94	Joback Method
cpg	565.23	J/mol×K	1052.64	Joback Method
cpg	570.92	J/mol×K	1091.35	Joback Method
hfust	40.40	kJ/mol	452.60	NIST Webbook
hfust	39.40	kJ/mol	454.20	NIST Webbook
hsubt	114.70 ± 1.30	kJ/mol	339.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15307865&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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