Chlorfenac

Other names:	(2,3,6-Trichlorophenyl)acetic acid
	2,3,6-Trichlorobenzeneacetic acid
	2,3,6-Trichlorphenylessigsaeure
	2-(2,3,6-trichlorophenyl)acetic acid
	Acetic acid, (2,3,6-trichlorophenyl)-
	Benzeneacetic acid, 2,3,6-trichloro-
	Fenac
	Fenae
	Fenatrol
	Kanepar
	Kyselina 2,3,6-trichlorfenyloctova
	NSC 41931
	TCPA
	Tri-Fen
	Tri-fene
Inchi:	InChI=1S/C8H5Cl3O2/c9-5-1-2-6(10)8(11)4(5)3-7(12)13/h1-2H,3H2,(H,12,13)
InchiKey:	QZXCCPZJCKEPSA-UHFFFAOYSA-N
Formula:	C8H5Cl3O2
SMILES:	O=C(O)Cc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	239.48
CAS:	85-34-7

Physical Properties

Property code	Value	Unit	Source
gf	-201.53	kJ/mol	Joback Method
hf	-318.36	kJ/mol	Joback Method
hfus	27.63	kJ/mol	Joback Method
hvap	74.24	kJ/mol	Joback Method
log10ws	-3.08		Aqueous Solubility Prediction Method
logp	3.274		Crippen Method
mcvol	143.980	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	682.40	K	Joback Method
tc	902.53	K	Joback Method
tf	431.65	K	Aqueous Solubility Prediction Method

tf	433.50 ± 0.20	K	NIST Webbook
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.00	J/mol×K	682.40	Joback Method
cpg	299.76	J/mol×K	719.09	Joback Method
cpg	306.04	J/mol×K	755.78	Joback Method
cpg	311.86	J/mol×K	792.47	Joback Method
cpg	317.23	J/mol×K	829.16	Joback Method
cpg	322.17	J/mol×K	865.85	Joback Method
cpg	326.71	J/mol×K	902.53	Joback Method
dvisc	0.0005779	Pa×s	484.07	Joback Method
dvisc	0.0010863	Pa×s	444.41	Joback Method
dvisc	0.0003383	Pa×s	523.74	Joback Method
dvisc	0.0002135	Pa×s	563.40	Joback Method
dvisc	0.0001432	Pa×s	603.07	Joback Method
dvisc	0.0001009	Pa×s	642.73	Joback Method
dvisc	0.0000740	Pa×s	682.40	Joback Method
hfust	22.43	kJ/mol	432.30	NIST Webbook
hfust	22.43	kJ/mol	432.30	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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85347&Units=SI

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

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
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

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