

Fenclofenac

Inchi:	InChI=1S/C14H10Cl2O3/c15-10-5-6-13(11(16)8-10)19-12-4-2-1-3-9(12)7-14(17)18/h1-6,
InchiKey:	IDKAXRLETRCXKS-UHFFFAOYSA-N
Formula:	C14H10Cl2O3
SMILES:	O=C(O)Cc1ccccc1Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	297.14

Physical Properties

Property code	Value	Unit	Source
gf	-131.67	kJ/mol	Joback Method
hf	-322.15	kJ/mol	Joback Method
hfus	34.20	kJ/mol	Joback Method
hvap	87.90	kJ/mol	Joback Method
log10ws	-3.85		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	4.413		Crippen Method
mcvol	198.390	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	831.35	K	Joback Method
tc	1062.22	K	Joback Method
tf	530.76	K	Joback Method
vc	0.745	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.55	J/mol×K	831.35	Joback Method
cpg	512.86	J/mol×K	869.83	Joback Method
cpg	521.31	J/mol×K	908.31	Joback Method
cpg	528.93	J/mol×K	946.78	Joback Method
cpg	535.75	J/mol×K	985.26	Joback Method
cpg	541.81	J/mol×K	1023.74	Joback Method
cpg	547.14	J/mol×K	1062.22	Joback Method
dvisc	0.0003362	Paxs	530.76	Joback Method

dvisc	0.0001763	Paxs	580.86	Joback Method
dvisc	0.0001024	Paxs	630.96	Joback Method
dvisc	0.0000645	Paxs	681.06	Joback Method
dvisc	0.0000432	Paxs	731.15	Joback Method
dvisc	0.0000305	Paxs	781.25	Joback Method
dvisc	0.0000225	Paxs	831.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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