Alclofenac

Other names:	3-Chloro-4-(2-propenyloxy)benzeneacetic acid
	Acetic acid, [4-(allyloxy)-3-chlorophenyl]-
	Alclophenac
	Allopydin
	Argun
	Benzeneacetic acid, 3-chloro-4-(2-propenyloxy)-
	Epinal
	Kyselina 4-allyloxy-3-chlorfenyloctova
	MY 101
	Medifenac
	Mervan
	Neosten
	Neoston
	Prinalgin
	Reufenac
	W 7320
	Zumaril
	[3-Chloro-4-(allyloxy)phenyl]acetic acid
	[4-(Allyloxy)-3-chlorophenyl]acetic acid
Inchi:	InChI=1S/C11H11ClO3/c1-2-5-15-10-4-3-8(6-9(10)12)7-11(13)14/h2-4,6H,1,5,7H2,(H,13
InchiKey:	ARHWPKZXBHOEEE-UHFFFAOYSA-N
Formula:	C11H11ClO3
SMILES:	C=CCOc1ccc(CC(=O)O)cc1Cl
Mol. weight [g/mol]:	226.66
CAS:	22131-79-9

Physical Properties

Property code	Value	Unit	Source
gf	-159.94	kJ/mol	Joback Method
hf	-344.12	kJ/mol	Joback Method
hfus	27.30	kJ/mol	Joback Method
hvap	73.23	kJ/mol	Joback Method
log10ws	-3.12		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	2.532		Crippen Method
mcvol	163.340	ml/mol	McGowan Method

pc	2986.06	kPa	Joback Method
rinpol	1837.00		NIST Webbook
tb	690.30	K	Joback Method
tc	895.12	K	Joback Method
tf	426.33	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.60	J/mol×K	690.30	Joback Method
cpg	408.64	J/mol×K	724.44	Joback Method
cpg	418.06	J/mol×K	758.57	Joback Method
cpg	426.86	J/mol×K	792.71	Joback Method
cpg	435.07	J/mol×K	826.85	Joback Method
cpg	442.71	J/mol×K	860.98	Joback Method
cpg	449.78	J/mol×K	895.12	Joback Method
dvisc	0.0011220	Pa×s	426.33	Joback Method
dvisc	0.0005239	Pa×s	470.32	Joback Method
dvisc	0.0002786	Pa×s	514.32	Joback Method
dvisc	0.0001637	Pa×s	558.32	Joback Method
dvisc	0.0001040	Pa×s	602.31	Joback Method
dvisc	0.0000702	Pa×s	646.31	Joback Method
dvisc	0.0000499	Pa×s	690.30	Joback Method

Sources

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=C22131799&Units=SI

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

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

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
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