Diclofenac, methyl ester

Other names:	Methyl [2-(2,6-dichloroanilino)phenyl]acetate
	Diclofenac, Me
	Diclofenac, methylated
	Acetic acid, [o-(2,6-dichloroanilino)phenyl]-, methyl ester
	Diclofenac, methyl deriv.
Inchi:	InChI=1S/C15H13Cl2NO2/c1-20-14(19)9-10-5-2-3-8-13(10)18-15-11(16)6-4-7-12(15)17/h
InchiKey:	VETACGBDFVVKGZ-UHFFFAOYSA-N
Formula:	C15H13Cl2NO2
SMILES:	COC(=O)Cc1ccccc1Nc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	310.18
CAS:	15307-78-5

Physical Properties

Property code	Value	Unit	Source
gf	102.96	kJ/mol	Joback Method
hf	-137.09	kJ/mol	Joback Method
hfus	37.80	kJ/mol	Joback Method
hvap	79.88	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.453		Crippen Method
mcvol	216.590	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	2200.00		NIST Webbook
tb	812.22	K	Joback Method
tc	1054.21	K	Joback Method
tf	533.87	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.49	J/mol×K	812.22	Joback Method
cpg	573.41	J/mol×K	852.55	Joback Method
cpg	584.23	J/mol×K	892.88	Joback Method

cpg	593.99	J/mol×K	933.22	Joback Method
cpg	602.75	J/mol×K	973.55	Joback Method
cpg	610.55	J/mol×K	1013.88	Joback Method
cpg	617.42	J/mol×K	1054.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15307785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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