Diclofenac, hydroxy, bis-methylated

Inchi: InChI=1S/C16H15Cl2NO3/c1-21-11-8-12(17)16(13(18)9-11)19-14-6-4-3-5-10(14)7-15(20
InchiKey: LMSWJSSPABTCQU-UHFFFAOYSA-N
Formula: C16H15Cl2NO3
SMILES: COC(=O)Cc1ccccc1Nc1c(Cl)cc(OC)cc1Cl
Mol. weight [g/mol]: 340.20

Physical Properties

Property code	Value	Unit	Source
gf	-3.25	kJ/mol	Joback Method
hf	-301.42	kJ/mol	Joback Method
hfus	41.19	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.461		Crippen Method
mcvol	236.550	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	2460.00		NIST Webbook
tb	862.50	K	Joback Method
tc	1098.70	K	Joback Method
tf	579.89	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.67	J/mol×K	862.50	Joback Method
cpg	651.25	J/mol×K	901.87	Joback Method
cpg	661.65	J/mol×K	941.23	Joback Method
cpg	670.89	J/mol×K	980.60	Joback Method
cpg	678.98	J/mol×K	1019.97	Joback Method
cpg	685.94	J/mol×K	1059.34	Joback Method
cpg	691.78	J/mol×K	1098.70	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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