Tolfenamic acid, methyl ester

Other names:	Methyl 2-(3-chloro-2-methylanilino)benzoate
	Tolfenamic acid, methyl deriv.
	Benzoic acid, 2-[(3-chloro-2-methylphenyl)amino]-, methyl ester
Inchi:	InChI=1S/C15H14ClNO2/c1-10-12(16)7-5-9-13(10)17-14-8-4-3-6-11(14)15(18)19-2/h3-9
InchiKey:	CNIPMLJEWLMTCO-UHFFFAOYSA-N
Formula:	C15H14ClNO2
SMILES:	COC(=O)c1ccccc1Nc1cccc(Cl)c1C
Mol. weight [g/mol]:	275.73
CAS:	31376-49-5

Physical Properties

Property code	Value	Unit	Source
gf	114.89	kJ/mol	Joback Method
hf	-121.35	kJ/mol	Joback Method
hfus	33.60	kJ/mol	Joback Method
hvap	75.50	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.179		Crippen Method
mcvol	204.350	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	2255.00		NIST Webbook
tb	774.79	K	Joback Method
tc	1014.61	K	Joback Method
tf	503.95	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.34	J/mol×K	774.79	Joback Method
cpg	552.54	J/mol×K	814.76	Joback Method
cpg	564.62	J/mol×K	854.73	Joback Method
cpg	575.62	J/mol×K	894.70	Joback Method
cpg	585.57	J/mol×K	934.67	Joback Method

cpg	594.52	J/mol×K	974.64	Joback Method
cpg	602.51	J/mol×K	1014.61	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=C31376495&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