Benzoic acid, 2-[(2,6-dichloro-3-methylphenyl)amino]-, methyl ester

Other names: Meclofenamic acid methyl derivative
Meclofenamic acid, methyl deriv.
Meclofenamic acid, methyl ester

Inchi: InChI=1S/C15H13Cl2NO2/c1-9-7-8-11(16)14(13(9)17)18-12-6-4-3-5-10(12)15(19)20-2/h

InchiKey: IZZWHVDZJOINFQ-UHFFFAOYSA-N

Formula: C15H13Cl2NO2

SMILES: COC(=O)c1ccccc1Nc1c(Cl)ccc(C)c1Cl

Mol. weight [g/mol]: 310.18

CAS: 3254-79-3

Physical Properties

Property code	Value	Unit	Source
gf	93.33	kJ/mol	Joback Method
hf	-148.56	kJ/mol	Joback Method
hfus	37.41	kJ/mol	Joback Method
hvap	80.55	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.832		Crippen Method
mcvol	216.590	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	2240.00		NIST Webbook
tb	817.20	K	Joback Method
tc	1059.91	K	Joback Method
tf	546.39	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.90	J/mol×K	817.20	Joback Method
cpg	571.72	J/mol×K	857.65	Joback Method
cpg	582.46	J/mol×K	898.10	Joback Method
cpg	592.15	J/mol×K	938.55	Joback Method
cpg	600.82	J/mol×K	979.01	Joback Method

cpg	608.50	J/mol×K	1019.46	Joback Method
cpg	615.23	J/mol×K	1059.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3254793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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