Benzoic acid, 2-[(2,3-dimethylphenyl)amino]-, methyl ester

Other names: Monomethyl derivative of mefenamic acid
Mefenamic acid methyl derivative
Mefenamic acid, methyl deriv.
Mefenamic acid, methyl ester

Inchi: InChI=1S/C16H17NO2/c1-11-7-6-10-14(12(11)2)17-15-9-5-4-8-13(15)16(18)19-3/h4-10,1

InchiKey: LCCVYZLUEHOBDC-UHFFFAOYSA-N

Formula: C16H17NO2

SMILES: COC(=O)c1ccccc1Nc1cccc(C)c1C

Mol. weight [g/mol]: 255.31

CAS: 1222-42-0

Physical Properties

Property code	Value	Unit	Source
gf	135.24	kJ/mol	Joback Method
hf	-126.25	kJ/mol	Joback Method
hfus	32.00	kJ/mol	Joback Method
hvap	73.34	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.834		Crippen Method
mcvol	206.200	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	2110.00		NIST Webbook
tb	760.24	K	Joback Method
tc	993.42	K	Joback Method
tf	485.30	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.14	J/mol×K	760.24	Joback Method
cpg	583.97	J/mol×K	799.10	Joback Method
cpg	597.64	J/mol×K	837.97	Joback Method
cpg	610.20	J/mol×K	876.83	Joback Method

cpg	621.67	J/mol×K	915.69	Joback Method
cpg	632.10	J/mol×K	954.55	Joback Method
cpg	641.52	J/mol×K	993.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1222420&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

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