Benzoic acid, 2-(methylamino)-, ethyl ester

Other names: ethyl 2-methylaminobenzoate
Inchi: InChI=1S/C10H13NO2/c1-3-13-10(12)8-6-4-5-7-9(8)11-2/h4-7,11H,3H2,1-2H3
InchiKey: WBSWYVBUGLBCOV-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: CCOC(=O)c1ccccc1NC
Mol. weight [g/mol]: 179.22
CAS: 35472-56-1

Physical Properties

Property code	Value	Unit	Source
gf	-8.43	kJ/mol	Joback Method
hf	-216.00	kJ/mol	Joback Method
hfus	23.19	kJ/mol	Joback Method
hvap	56.38	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.905		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
tb	586.32	K	Joback Method
tc	800.02	K	Joback Method
tf	366.22	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.62	J/mol×K	586.32	Joback Method
cpg	360.93	J/mol×K	621.94	Joback Method
cpg	373.47	J/mol×K	657.55	Joback Method
cpg	385.26	J/mol×K	693.17	Joback Method
cpg	396.32	J/mol×K	728.79	Joback Method
cpg	406.66	J/mol×K	764.40	Joback Method
cpg	416.30	J/mol×K	800.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.70	K	6.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35472561&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume