

Benzoic acid, 3-(ethylamino)-, methyl ester

Inchi:	InChI=1S/C10H13NO2/c1-3-11-9-6-4-5-8(7-9)10(12)13-2/h4-7,11H,3H2,1-2H3
InchiKey:	SVZKZMCIAJUDGI-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCNc1cccc(C(=O)OC)c1
Mol. weight [g/mol]:	179.22

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
rinpola	1611.00		NIST Webbook
tb	586.32	K	Joback Method
tc	800.02	K	Joback Method
tf	366.22	K	Joback Method
vc	0.546	m ³ /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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374475&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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