

3-Ethoxybenzamide

Other names:	3-Ethoxybenzamide Benzoic amide, 3-ethoxy- m-ethoxybenzamide
Inchi:	InChI=1S/C9H11NO2/c1-2-12-8-5-3-4-7(6-8)9(10)11/h3-6H,2H2,1H3,(H2,10,11)
InchiKey:	NDOYNKFWOCOOIR-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CCOc1cccc(C(N)=O)c1
Mol. weight [g/mol]:	165.19

Physical Properties

Property code	Value	Unit	Source
af	0.6435		Cheméo Relay (1.0)
hf	-333.64	kJ/mol	Cheméo Relay (1.0)
hfus	20.70	kJ/mol	Joback Method
hvap	73.97	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-2.36		Cheméo Relay (1.0)
logp	1.184		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
tb	568.68	K	Cheméo Relay (1.0)
tc	767.83	K	Cheméo Relay (1.0)
tf	347.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.15	J/mol×K	585.80	Joback Method
cpg	322.35	J/mol×K	623.52	Joback Method
cpg	333.81	J/mol×K	661.24	Joback Method
cpg	344.53	J/mol×K	698.96	Joback Method
cpg	354.54	J/mol×K	736.68	Joback Method
cpg	363.84	J/mol×K	774.40	Joback Method
cpg	372.45	J/mol×K	812.12	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55836696&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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