2-ETHOXYBENZYLAMINE

Other names: Benzenemethanamine, 2-ethoxy-
2-Ethoxybenzylamine
Inchi: InChI=1S/C9H13NO/c1-2-11-9-6-4-3-5-8(9)7-10/h3-6H,2,7,10H2,1H3
InchiKey: LAUPTNYHVCVPFH-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: CCOc1ccccc1CN
Mol. weight [g/mol]: 151.21

Physical Properties

Property code	Value	Unit	Source
af	0.5149		Cheméo Relay (1.0)
hf	-133.05	kJ/mol	Cheméo Relay (1.0)
hfus	19.10	kJ/mol	Joback Method
hvap	63.55	kJ/mol	Cheméo Relay (1.0)
ie	8.01	eV	Cheméo Relay (1.0)
log10ws	-1.53		Cheméo Relay (1.0)
logp	1.544		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	510.61	K	Cheméo Relay (1.0)
tc	713.57	K	Cheméo Relay (1.0)
tf	292.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.02	J/mol×K	531.93	Joback Method
cpg	308.41	J/mol×K	568.29	Joback Method
cpg	321.08	J/mol×K	604.65	Joback Method
cpg	333.04	J/mol×K	641.01	Joback Method
cpg	344.32	J/mol×K	677.37	Joback Method
cpg	354.92	J/mol×K	713.73	Joback Method
cpg	364.86	J/mol×K	750.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.70	K	0.03	NIST Webbook

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=C37806294&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point