

N-Ethyl-2-phenethylamine

Other names:	N-ethylbenzeneethanamine
Inchi:	InChI=1S/C10H15N/c1-2-11-9-8-10-6-4-3-5-7-10/h3-7,11H,2,8-9H2,1H3
InchiKey:	WOHOHPONCSKXSQ-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CCNCCc1ccccc1
Mol. weight [g/mol]:	149.23
CAS:	22002-68-2

Physical Properties

Property code	Value	Unit	Source
gf	235.12	kJ/mol	Joback Method
hf	40.27	kJ/mol	Joback Method
hfus	20.80	kJ/mol	Joback Method
hvap	46.57	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.839		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	505.05	K	Joback Method
tc	711.40	K	Joback Method
tf	281.54	K	Joback Method
vc	0.522	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.53	J/molxK	505.05	Joback Method
cpg	319.73	J/molxK	539.44	Joback Method
cpg	334.07	J/molxK	573.83	Joback Method
cpg	347.57	J/molxK	608.22	Joback Method
cpg	360.27	J/molxK	642.61	Joback Method
cpg	372.21	J/molxK	677.00	Joback Method
cpg	383.43	J/molxK	711.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22002682&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
h vap:	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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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