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]: 149.24

Physical Properties

Property code	Value	Unit	Source
af	0.4414		Cheméo Relay (1.0)
gf	235.12	kJ/mol	Joback Method
hf	61.52	kJ/mol	Cheméo Relay (1.0)
hfus	20.80	kJ/mol	Joback Method
hvap	58.81	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
log10ws	-0.99		Cheméo Relay (1.0)
logp	1.839		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	496.49	K	Cheméo Relay (1.0)
tc	685.88	K	Cheméo Relay (1.0)
tf	257.70	K	Cheméo Relay (1.0)
vc	0.502	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

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=C22002682&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
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
vc:	Critical Volume