

3-(Ethylamino)phenol

Inchi:	InChI=1S/C8H11NO/c1-2-9-7-4-3-5-8(10)6-7/h3-6,9-10H,2H2,1H3
InchiKey:	TVKZDKSHNITMRZ-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	CCNc1cccc(O)c1
Mol. weight [g/mol]:	137.18
CAS:	621-31-8

Physical Properties

Property code	Value	Unit	Source
af	0.5924		Cheméo Relay (1.0)
gf	63.66	kJ/mol	Joback Method
hf	-126.04	kJ/mol	Cheméo Relay (1.0)
hfus	21.40	kJ/mol	Joback Method
hvap	78.94	kJ/mol	Cheméo Relay (1.0)
ie	7.46	eV	Cheméo Relay (1.0)
log10ws	-1.64		Cheméo Relay (1.0)
logp	1.824		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	550.90	K	Cheméo Relay (1.0)
tc	783.89	K	Cheméo Relay (1.0)
tf	335.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.389	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-4.84190e+01
Coeff. B	9.15720e-01

Coeff. C	-7.47560e-04
Coeff. D	2.53100e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
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

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

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