

Benzenemethanamine, N-ethyl-

Other names:	Benzylamine, N-ethyl- Benzylethylamine Ethylbenzylamine N-Benzyl-N-ethylamine N-Benzylethylamine N-Ethylbenzylamine
Inchi:	InChI=1S/C9H13N/c1-2-10-8-9-6-4-3-5-7-9/h3-7,10H,2,8H2,1H3
InchiKey:	HVAAHUDGWQAAOJ-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CCNCc1ccccc1
Mol. weight [g/mol]:	135.21
CAS:	14321-27-8

Physical Properties

Property code	Value	Unit	Source
chl	-5391.50	kJ/mol	NIST Webbook
gf	226.70	kJ/mol	Joback Method
hf	60.91	kJ/mol	Joback Method
hfl	-36.00	kJ/mol	NIST Webbook
hfus	18.21	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.796		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1120.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1103.50		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1577.00		NIST Webbook
tb	465.70	K	NIST Webbook
tc	691.55	K	Joback Method
tf	270.27	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.33	J/molxK	482.17	Joback Method
cpg	274.63	J/molxK	517.07	Joback Method
cpg	288.10	J/molxK	551.96	Joback Method
cpg	300.77	J/molxK	586.86	Joback Method
cpg	312.68	J/molxK	621.76	Joback Method
cpg	323.85	J/molxK	656.66	Joback Method
cpg	334.34	J/molxK	691.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47811e+01
Coeff. B	-4.01105e+03
Coeff. C	-7.10180e+01
Temperature range (K), min.	347.77
Temperature range (K), max.	494.59

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method:

https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method:

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C14321278&Units=SI>

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	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
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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