

Benzenemethanamine, N-ethyl-N-(3-methylphenyl)-

Other names:	m-Toluidine, N-benzyl-N-ethyl- 3-(N-Benzyl-N-ethylamino)methylbenzene 3-(N-Benzyl-N-ethylamino)toluene N-Benzyl-N-ethyl-meta-toluidine N-Ethyl-N-benzyl-m-toluidine N-Ethyl-N-benzyl-meta-toluidine N-Benzyl-N-ethyl-m-toluidine
Inchi:	InChI=1S/C16H19N/c1-3-17(13-15-9-5-4-6-10-15)16-11-7-8-14(2)12-16/h4-12H,3,13H2,1
InchiKey:	VIACAIAQHPLINF-UHFFFAOYSA-N
Formula:	C16H19N
SMILES:	CCN(Cc1ccccc1)c1cccc(C)c1
Mol. weight [g/mol]:	225.33
CAS:	119-94-8

Physical Properties

Property code	Value	Unit	Source
gf	409.81	kJ/mol	Joback Method
hf	155.55	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	58.47	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.022		Crippen Method
mcvol	198.760	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
tb	636.26	K	Joback Method
tc	863.58	K	Joback Method
tf	367.91	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	510.36	J/mol×K	636.26	Joback Method
cpg	529.00	J/mol×K	674.15	Joback Method
cpg	546.32	J/mol×K	712.03	Joback Method
cpg	562.39	J/mol×K	749.92	Joback Method
cpg	577.28	J/mol×K	787.80	Joback Method
cpg	591.08	J/mol×K	825.69	Joback Method
cpg	603.86	J/mol×K	863.58	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119948&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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