N-(m-Tolyl)-diethanolamine

Other names:	N,N-Bis-(hydroxyethyl)-m-toluidine N,N-Bis(2-hydroxyethyl)-m-toluidine m-Tolyl diethanolamine Ethanol, 2,2'-[(3-methylphenyl)imino]bis- m-Tolydiethanolamine Diethanol-m-toluidine Ethanol, 2,2'-(m-tolylimino)di- MTDEA N,N-Bis(2-hydroxyethyl)-3-methylaniline N,N-Di(hydroxyethyl)-m-toluidine 2,2'-(m-Tolylimino)diethanol N,N-Bis(«beta»-hydroxyethyl)-3-methylaniline Emery 5709 m-Toluidine, N,N-bis(2-hydroxyethyl)- N,N-Di(2-hydroxyethyl)-m-toluidine NSC 7488
Inchi:	InChI=1S/C11H17NO2/c1-10-3-2-4-11(9-10)12(5-7-13)6-8-14/h2-4,9,13-14H,5-8H2,1H3
InchiKey:	VMNDRLYLEVCGAG-UHFFFAOYSA-N
Formula:	C11H17NO2
SMILES:	Cc1cccc(N(CCO)CCO)c1
Mol. weight [g/mol]:	195.26
CAS:	91-99-6

Physical Properties

Property code	Value	Unit	Source
gf	-18.34	kJ/mol	Joback Method
hf	-282.24	kJ/mol	Joback Method
hfus	29.10	kJ/mol	Joback Method
hvap	78.42	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	0.786		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
tb	679.54	K	Joback Method
tc	861.10	K	Joback Method
tf	406.78	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.02	J/mol×K	679.54	Joback Method
cpg	460.21	J/mol×K	709.80	Joback Method
cpg	470.78	J/mol×K	740.06	Joback Method
cpg	480.77	J/mol×K	770.32	Joback Method
cpg	490.20	J/mol×K	800.58	Joback Method
cpg	499.11	J/mol×K	830.84	Joback Method
cpg	507.53	J/mol×K	861.10	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C91996&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume