N-Ethyl trimethylene diamine

Inchi: InChI=1S/C5H14N2/c1-2-7-5-3-4-6/h7H,2-6H2,1H3
InchiKey: ODGYWRBCQWKSSH-UHFFFAOYSA-N
Formula: C5H14N2
SMILES: CCNCCCN
Mol. weight [g/mol]: 102.18

Physical Properties

Property code	Value	Unit	Source
af	0.4911		Cheméo Relay (1.0)
gf	147.06	kJ/mol	Joback Method
hf	-86.28	kJ/mol	Cheméo Relay (1.0)
hfus	19.00	kJ/mol	Joback Method
hvap	47.71	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
log10ws	0.63		Cheméo Relay (1.0)
logp	-0.055		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	422.94	K	Cheméo Relay (1.0)
tc	597.39	K	Cheméo Relay (1.0)
tf	227.06	K	Cheméo Relay (1.0)
vc	0.366	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.90	J/mol×K	436.50	Joback Method
cpg	224.78	J/mol×K	467.40	Joback Method
cpg	235.20	J/mol×K	498.30	Joback Method
cpg	245.17	J/mol×K	529.20	Joback Method
cpg	254.70	J/mol×K	560.10	Joback Method
cpg	263.81	J/mol×K	591.00	Joback Method
cpg	272.50	J/mol×K	621.90	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=C38571878&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