

Bis(hexamethylene)triamine

Inchi:	InChI=1S/C12H29N3/c13-9-5-1-3-7-11-15-12-8-4-2-6-10-14/h15H,1-14H2
InchiKey:	MRNZSTM RDWRNNR-UHFFFAOYSA-N
Formula:	C12H29N3
SMILES:	NCCCCCNCCCCCN
Mol. weight [g/mol]:	215.39
CAS:	143-23-7

Physical Properties

Property code	Value	Unit	Source
hf	-218.47	kJ/mol	Cheméo Relay (1.0)
hfus	42.33	kJ/mol	Joback Method
hvap	92.18	kJ/mol	Cheméo Relay (1.0)
ie	7.90	eV	Cheméo Relay (1.0)
log10ws	-2.23		Cheméo Relay (1.0)
logp	1.614		Crippen Method
mcvol	209.880	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
tb	589.46	K	Cheméo Relay (1.0)
tc	772.85	K	Cheméo Relay (1.0)
tf	306.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

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	3.75200e+00
Coeff. B	1.34380e+00
Coeff. C	-7.64400e-04
Coeff. D	1.64100e-07
Coeff. E	0.00000e+00

Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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):	
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

Legend

cpg:	Ideal gas heat capacity
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

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