

3-CYCLOHEXENE-1-METHANAMINE, .ALPHA.,.ALPHA.,4-TRIMETHYL-

Other names: a,a,4-Trimethyl-cyclohex-3-ene-1-methanamine
Inchi: InChI=1S/C10H19N/c1-8-4-6-9(7-5-8)10(2,3)11/h4,9H,5-7,11H2,1-3H3
InchiKey: LAVSBOJEEKTASF-UHFFFAOYSA-N
Formula: C10H19N
SMILES: CC1=CCC(C(C)(C)N)CC1
Mol. weight [g/mol]: 153.27

Physical Properties

Property code	Value	Unit	Source
hf	-50.85	kJ/mol	Cheméo Relay (1.0)
hfus	12.11	kJ/mol	Joback Method
hvap	54.87	kJ/mol	Cheméo Relay (1.0)
ie	7.76	eV	Cheméo Relay (1.0)
log10ws	-2.63		Cheméo Relay (1.0)
logp	2.470		Crippen Method
mcvol	146.580	ml/mol	McGowan Method
rinpol	1187.00		NIST Webbook
tb	472.96	K	Cheméo Relay (1.0)
tf	253.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.03	J/mol×K	521.19	Joback Method
cpg	375.17	J/mol×K	558.75	Joback Method
cpg	393.09	J/mol×K	596.31	Joback Method
cpg	409.84	J/mol×K	633.87	Joback Method
cpg	425.47	J/mol×K	671.43	Joback Method
cpg	440.05	J/mol×K	708.99	Joback Method
cpg	453.62	J/mol×K	746.56	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=C64374238&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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