

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]:	153.26
CAS:	64374-23-8

Physical Properties

Property code	Value	Unit	Source
gf	147.39	kJ/mol	Joback Method
hf	-124.06	kJ/mol	Joback Method
hfus	12.11	kJ/mol	Joback Method
hvap	48.58	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.470		Crippen Method
mcvol	146.580	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	1187.00		NIST Webbook
tb	521.19	K	Joback Method
tc	746.56	K	Joback Method
tf	308.80	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.03	J/molxK	521.19	Joback Method
cpg	375.17	J/molxK	558.75	Joback Method
cpg	393.09	J/molxK	596.31	Joback Method
cpg	409.84	J/molxK	633.87	Joback Method
cpg	425.47	J/molxK	671.43	Joback Method
cpg	440.05	J/molxK	708.99	Joback Method
cpg	453.62	J/molxK	746.56	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=C64374238&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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