

2-METHYLCYCLOHEXYLAMINE

Other names:	2-Methylcyclohexylamine,c&t Cyclohexanamine, 2-methyl- o-Methylcyclohexylamine Cyclohexylamine, 2-methyl- 2-Methylcyclohexanamine
Inchi:	InChI=1S/C7H15N/c1-6-4-2-3-5-7(6)8/h6-7H,2-5,8H2,1H3
InchiKey:	FEUISMYEFPANSS-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	CC1CCCCC1N
Mol. weight [g/mol]:	113.20

Physical Properties

Property code	Value	Unit	Source
af	0.3126		Cheméo Relay (1.0)
gf	91.25	kJ/mol	Joback Method
hf	-124.36	kJ/mol	Cheméo Relay (1.0)
hfus	11.99	kJ/mol	Joback Method
hvap	45.71	kJ/mol	Cheméo Relay (1.0)
ie	8.38	eV	Cheméo Relay (1.0)
log10ws	-2.04		Cheméo Relay (1.0)
logp	1.524		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	416.87	K	Cheméo Relay (1.0)
tc	631.21	K	Cheméo Relay (1.0)
tf	225.38	K	Cheméo Relay (1.0)
vc	0.373	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.34	J/mol×K	446.97	Joback Method
cpg	250.45	J/mol×K	483.23	Joback Method
cpg	266.69	J/mol×K	519.48	Joback Method

cpg	282.07	J/mol×K	555.74	Joback Method
cpg	296.61	J/mol×K	591.99	Joback Method
cpg	310.34	J/mol×K	628.25	Joback Method
cpg	323.26	J/mol×K	664.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7003329&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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

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