

Cyclohexanone, 2-(dimethylamino)-

Other names:	2-(Dimethylamino)cyclohexanone 2-(N,N-Dimethylamino)cyclohexanone
Inchi:	InChI=1S/C8H15NO/c1-9(2)7-5-3-4-6-8(7)10/h7H,3-6H2,1-2H3
InchiKey:	JOZKRRZOWRUDEK-UHFFFAOYSA-N
Formula:	C8H15NO
SMILES:	CN(C)C1CCCCC1=O
Mol. weight [g/mol]:	141.21
CAS:	6970-60-1

Physical Properties

Property code	Value	Unit	Source
gf	29.12	kJ/mol	Joback Method
hf	-224.30	kJ/mol	Joback Method
hfus	10.84	kJ/mol	Joback Method
hvap	40.12	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	1.060		Crippen Method
mcvol	124.270	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
tb	482.25	K	Joback Method
tc	699.42	K	Joback Method
tf	287.99	K	Joback Method
vc	0.442	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.65	J/mol×K	482.25	Joback Method
cpg	297.52	J/mol×K	518.44	Joback Method
cpg	314.52	J/mol×K	554.64	Joback Method
cpg	330.65	J/mol×K	590.83	Joback Method
cpg	345.93	J/mol×K	627.03	Joback Method
cpg	360.34	J/mol×K	663.22	Joback Method
cpg	373.90	J/mol×K	699.42	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.00 ± 1.00	K	2.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6970601&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvap:	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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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