

2,3-Dimethylcyclohexylamine

Other names:	Cyclohexanamine, 2,3-dimethyl-
Inchi:	InChI=1S/C8H17N/c1-6-4-3-5-8(9)7(6)2/h6-8H,3-5,9H2,1-2H3
InchiKey:	LKWOOKWVBNLSGN-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	CC1CCCC(N)C1C
Mol. weight [g/mol]:	127.23
CAS:	42195-92-6

Physical Properties

Property code	Value	Unit	Source
gf	91.96	kJ/mol	Joback Method
hf	-161.02	kJ/mol	Joback Method
hfus	15.65	kJ/mol	Joback Method
hvap	43.85	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.770		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	432.20	K	NIST Webbook
tc	679.35	K	Joback Method
tf	262.08	K	Joback Method
vc	0.444	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.53	J/molxK	465.18	Joback Method
cpg	296.02	J/molxK	500.87	Joback Method
cpg	313.61	J/molxK	536.57	Joback Method
cpg	330.32	J/molxK	572.26	Joback Method
cpg	346.15	J/molxK	607.96	Joback Method
cpg	361.13	J/molxK	643.65	Joback Method
cpg	375.26	J/molxK	679.35	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44427e+01
Coeff. B	-3.64398e+03
Coeff. C	-6.12880e+01
Temperature range (K), min.	318.72
Temperature range (K), max.	460.36

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42195926&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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