3-Methylcyclohexylamine,c&t

Other names:	3-Methylcyclohexylamine
	3-Methylcyclohexylamine, (cis+trans)
	3-methylcyclohexylamine, mixed isomers
	Cyclohexanamine, 3-methyl-
Inchi:	InChI=1S/C7H15N/c1-6-3-2-4-7(8)5-6/h6-7H,2-5,8H2,1H3
InchiKey:	JYDYHSHPBDZRPU-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	CC1CCCC(N)C1
Mol. weight [g/mol]:	113.20
CAS:	6850-35-7

Physical Properties

Property code	Value	Unit	Source
chl	-4718.30	kJ/mol	NIST Webbook
gf	91.25	kJ/mol	Joback Method
hf	-120.04	kJ/mol	Joback Method
hfus	11.99	kJ/mol	Joback Method
hvap	41.94	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.524		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	926.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	926.00		NIST Webbook
ripol	1231.00		NIST Webbook
ripol	1231.00		NIST Webbook
ripol	1231.00		NIST Webbook
tb	446.97	K	Joback Method
tc	664.51	K	Joback Method
tf	255.05	K	Joback Method
vc	0.389	m3/kmol	Joback Method

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51825e+01
Coeff. B	-3.76445e+03
Coeff. C	-5.87860e+01
Temperature range (K), min.	311.52
Temperature range (K), max.	440.15

Sources

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=C6850357&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume