3-METHYLCYCLOHEXYLAMINE

Other names: 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
af	0.3189		Cheméo Relay (1.0)
chl	-4718.30	kJ/mol	NIST Webbook
gf	91.25	kJ/mol	Joback Method
hf	-113.58	kJ/mol	Cheméo Relay (1.0)
hfus	11.99	kJ/mol	Joback Method
hvap	45.11	kJ/mol	Cheméo Relay (1.0)
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-2.21		Cheméo Relay (1.0)
logp	1.524		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
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
rinpol	926.00		NIST Webbook
ripol	1231.00		NIST Webbook
ripol	1231.00		NIST Webbook
ripol	1231.00		NIST Webbook
tb	416.59	K	Cheméo Relay (1.0)
tc	626.72	K	Cheméo Relay (1.0)
tf	207.75	K	Cheméo Relay (1.0)
vc	0.375	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

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

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6850357&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.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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