

Cyclohexane, isocyanato-

Other names:	Cyclohexyl ester of isocyanic acid Cyclohexyl isocyanate Cyclohexylisocyanate ISOCYANATOCYCLOHEXANE Isocyanic acid, cyclohexyl ester NSC 87419 UN 2488
Inchi:	InChI=1S/C7H11NO/c9-6-8-7-4-2-1-3-5-7/h7H,1-5H2
InchiKey:	KQWGXHWJMSMDJJ-UHFFFAOYSA-N
Formula:	C7H11NO
SMILES:	O=C=NC1CCCCC1
Mol. weight [g/mol]:	125.17
CAS:	3173-53-3

Physical Properties

Property code	Value	Unit	Source
hf	-138.90	kJ/mol	Joback Method
hvap	41.14	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	1.655		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	1216.00		NIST Webbook
tb	445.78	K	Joback Method
tc	661.40	K	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.14239e+01
Coeff. B	-3.06420e+03
Coeff. C	-5.55420e+01

Temperature range (K), min.	330.70
Temperature range (K), max.	556.85

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	8.62857e+01
Coeff. B	-9.28830e+03
Coeff. C	-1.00888e+01
Coeff. D	3.97323e-06
Temperature range (K), min.	193.00
Temperature range (K), max.	633.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1475.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3173533&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1475
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

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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