Methane, isocyanato-

Other names:	CH3NCO
	ISO-CYANOMETHANE
	ISOCYANATOMETHANE
	Isocyanate de methyle
	Isocyanic acid, methyl ester
	METHYL CARBONIMIDE
	MIC
	Methyl isocyanat
	Methyl isocyanate
	Methylisocyanaat
	Methylisokyanat
	Metil isocianato
	NSC 64323
	Rcra waste number P064
	TL 1450
	UN 2480
Inchi:	InChI=1S/C2H3NO/c1-3-2-4/h1H3
InchiKey:	HAMGRBXTJNITHG-UHFFFAOYSA-N
Formula:	C2H3NO
SMILES:	CN=C=O
Mol. weight [g/mol]:	57.05
CAS:	624-83-9

Physical Properties

Property code	Value	Unit	Source
af	0.2780		KDB
affp	764.40	kJ/mol	NIST Webbook
basg	732.00	kJ/mol	NIST Webbook
hf	-90.00	kJ/mol	KDB
hvap	29.58	kJ/mol	Joback Method
ie	10.67 ± 0.02	eV	NIST Webbook
log10ws	-4.16		Crippen Method
logp	-0.048		Crippen Method
mcvol	46.290	ml/mol	McGowan Method
pc	5570.00	kPa	KDB
rinpol	96.70		NIST Webbook
rinpol	502.00		NIST Webbook

rinpol	502.00		NIST Webbook
tb	312.00	K	KDB
tb	312.25	K	NIST Webbook
tc	491.00	K	KDB
tt	178.46	K	Entropy, related thermodynamic properties, and structure of methylisocyanate

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	29.90	kJ/mol	286.50	NIST Webbook
hvapt	31.70	kJ/mol	281.50	NIST Webbook
rhol	958.00	kg/m3	293.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34035e+01
Coeff. B	-2.10799e+03
Coeff. C	-7.23020e+01
Temperature range (K), min.	233.02
Temperature range (K), max.	332.80

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.55185e+02
Coeff. B	-8.94924e+03
Coeff. C	-2.15877e+01
Coeff. D	2.14699e-05
Temperature range (K), min.	230.00
Temperature range (K), max.	505.00

Sources

Entropy, related thermodynamic properties, and structure of methylisocyanate:	https://www.doi.org/10.1016/j.jct.2012.10.011
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1458.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624839&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1458
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tt:	Triple Point Temperature