

Octane, 1-isocyanato-

Other names:	1-Octyl isocyanate Isocyanic acid, octyl ester Octyl isocyanate n-Octyl isocyanate
Inchi:	InChI=1S/C9H17NO/c1-2-3-4-5-6-7-8-10-9-11/h2-8H2,1H3
InchiKey:	DYQFCTCUULUMTQ-UHFFFAOYSA-N
Formula:	C9H17NO
SMILES:	CCCCCCCCN=C=O
Mol. weight [g/mol]:	155.24
CAS:	3158-26-7

Physical Properties

Property code	Value	Unit	Source
hf	-234.50	kJ/mol	Joback Method
hvap	45.16	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	2.683		Crippen Method
mvol	144.920	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	471.99	K	Joback Method
tc	646.08	K	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43429e+01
Coeff. B	-4.07432e+03
Coeff. C	-7.32420e+01
Temperature range (K), min.	363.12
Temperature range (K), max.	524.37

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3158267&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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