

Benzene, isocyanato-

Other names:	Additive T1 CARBANIL Fenylisokyanat ISOCYANATOBENZENE Isocyanic acid, phenyl ester Karbanil Mondur P NSC 74454 PHENYL CARBONIMIDE Phenyl ester of isocyanic acid Phenyl isocyanate Phenylcarbimide UN 2487
Inchi:	InChI=1S/C7H5NO/c9-6-8-7-4-2-1-3-5-7/h1-5H
InchiKey:	DGTNSSLYPYDJGL-UHFFFAOYSA-N
Formula:	C7H5NO
SMILES:	O=C=Nc1ccccc1
Mol. weight [g/mol]:	119.12
CAS:	103-71-9

Physical Properties

Property code	Value	Unit	Source
chl	-3455.10 ± 1.30	kJ/mol	NIST Webbook
chl	-3402.00	kJ/mol	NIST Webbook
chl	-3408.07 ± 0.85	kJ/mol	NIST Webbook
hf	-14.50 ± 1.20	kJ/mol	NIST Webbook
hf	-22.10	kJ/mol	NIST Webbook
hfl	-33.90 ± 1.30	kJ/mol	NIST Webbook
hfl	-61.10 ± 1.10	kJ/mol	NIST Webbook
hfl	-33.90 ± 1.30	kJ/mol	NIST Webbook
hvap	45.00	kJ/mol	NIST Webbook
hvap	46.50 ± 0.30	kJ/mol	NIST Webbook
hvap	46.50 ± 0.30	kJ/mol	NIST Webbook
ie	8.77 ± 0.02	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	8.77 ± 0.02	eV	NIST Webbook
ie	8.80	eV	NIST Webbook

ie	9.20	eV	NIST Webbook
log10ws	-5.95		Crippen Method
logp	1.654		Crippen Method
mcvol	92.980	ml/mol	McGowan Method
pc	4540.00 ± 300.00	kPa	NIST Webbook
pc	4000.00	kPa	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method
rhoc	348.79 ± 20.25	kg/m ³	NIST Webbook
rinpol	142.80		NIST Webbook
rinpol	142.80		NIST Webbook
tb	452.91	K	Joback Method
tc	675.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	186.20	J/mol×K	298.15	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55620e+01
Coeff. B	-4.48522e+03
Coeff. C	-2.90940e+01
Temperature range (K), min.	322.74
Temperature range (K), max.	466.65

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	6.19158e+01
Coeff. B	-7.31927e+03
Coeff. C	-6.80993e+00

Coeff. D	4.24507e-06
Temperature range (K), min.	243.15
Temperature range (K), max.	648.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1474
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1474.mol
Critical Point and Vapor Pressure Measurements for 17 Compounds by a Crippen Method:	https://www.doi.org/10.1021/je060269j
Low Pressure Time Flow Method:	https://www.chemed.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103719&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation 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
rhoc:	Critical density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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