

Hexane, 1,6-diisocyanato-

Other names: Isocyanic acid, hexamethylene ester
Hexamethylene diisocyanate
Hexane 1,6-diisocyanate
1,6-Diisocyanatohexane
1,6-Hexamethylene diisocyanate
1,6-Hexylene diisocyanate
Hexamethylene 1,6-diisocyanate
HMDI
Isocyanic acid, diester with 1,6-hexanediol
Metyleno-bis-fenyloizocyjanian
Szesciometylenodwuizocyjanian
TL 78
HDI
NSC 11687

Inchi: InChI=1S/C8H12N2O2/c11-7-9-5-3-1-2-4-6-10-8-12/h1-6H2

InchiKey: RRAMGCGOFNQTLD-UHFFFAOYSA-N

Formula: C8H12N2O2

SMILES: O=C=NCCCCCN=C=O

Mol. weight [g/mol]: 168.19

CAS: 822-06-0

Physical Properties

Property code	Value	Unit	Source
hf	-219.27	kJ/mol	Joback Method
hvap	52.47	kJ/mol	Joback Method
log10ws	-10.17		Crippen Method
logp	1.218		Crippen Method
mcvol	138.080	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
sl	420.10	J/mol×K	NIST Webbook
tb	515.78	K	Joback Method
tc	700.81	K	Joback Method
tt	206.06 ± 0.01	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	294.00	J/mol×K	298.15	NIST Webbook
cpl	294.00	J/mol×K	298.15	NIST Webbook
cpl	299.20	J/mol×K	298.00	NIST Webbook
hfust	18.64	kJ/mol	206.06	NIST Webbook
hfust	18.64	kJ/mol	206.06	NIST Webbook
hfust	18.64	kJ/mol	206.10	NIST Webbook
sfust	90.46	J/mol×K	206.06	NIST Webbook
sfust	90.46	J/mol×K	206.06	NIST Webbook

Sources

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=C822060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tt:	Triple Point Temperature

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