n-Heptyl isocyanate

Other names: Heptyl isocyanate
Inchi: InChI=1S/C8H15NO/c1-2-3-4-5-6-7-9-8-10/h2-7H2,1H3
InchiKey: RFXBSYPBSRSQDU-UHFFFAOYSA-N
Formula: C8H15NO
SMILES: CCCCCCCN=C=O
Mol. weight [g/mol]: 141.21
CAS: 4747-81-3

Physical Properties

Property code	Value	Unit	Source
hf	-213.86	kJ/mol	Joback Method
hvap	42.93	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	2.293		Crippen Method
mcvol	130.830	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	449.11	K	Joback Method
tc	624.56	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	47.50	kJ/mol	393.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56173e+01
Coeff. B	-4.39733e+03

Coeff. C	-7.16290e+01
Temperature range (K), min.	358.48
Temperature range (K), max.	498.31

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=C4747813&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
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature