

Dodecane, 1-isocyanato-

Other names:	Dodecyl isocyanate
Inchi:	InChI=1S/C13H25NO/c1-2-3-4-5-6-7-8-9-10-11-12-14-13-15/h2-12H2,1H3
InchiKey:	YIDSTEJLDQMWBR-UHFFFAOYSA-N
Formula:	C13H25NO
SMILES:	CCCCCCCCCCCCN=C=O
Mol. weight [g/mol]:	211.34
CAS:	4202-38-4

Physical Properties

Property code	Value	Unit	Source
hf	-317.06	kJ/mol	Joback Method
hvap	54.06	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	4.243		Crippen Method
mcvol	201.280	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
tb	563.51	K	Joback Method
tc	732.56	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4202384&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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