

Dicyclohexylcarbodiimide

Other names:	Cyclohexanamine, N,N'-methanetetraylbis-1,3-Dicyclohexylcarbodiimide Carbodiimide, dicyclohexyl- Carbodicyclohexylimide DCC DCCD DCCI N,N'-Dicyclohexylcarbodiimide N,N'-Methanetetraylbiscyclohexanamine Methanediimine, N,N'-dicyclohexyl- Bis(cyclohexyl)carbodiimide NSC 30022
Inchi:	InChI=1S/C13H22N2/c1-3-7-12(8-4-1)14-11-15-13-9-5-2-6-10-13/h12-13H,1-10H2
InchiKey:	QOSSAOTZNIDXMA-UHFFFAOYSA-N
Formula:	C13H22N2
SMILES:	<chem>C(=NC1CCCCC1)=NC1CCCCC1</chem>
Mol. weight [g/mol]:	206.33
CAS:	538-75-0

Physical Properties

Property code	Value	Unit	Source
hf	6.99	kJ/mol	Joback Method
hvap	52.50	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.826		Crippen Method
mcpvol	183.670	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
tb	688.41	K	Joback Method
tc	950.73	K	Joback Method

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=C538750&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

hf: Enthalpy of formation at standard conditions
h_{vap}: Enthalpy of vaporization at standard conditions
log₁₀ws: Log₁₀ of Water solubility in mol/l
log_p: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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