

Decamethylene diisocyanate

Inchi: InChI=1S/C12H20N2O2/c15-11-13-9-7-5-3-1-2-4-6-8-10-14-12-16/h1-10H2
InchiKey: VNMOIBZLSJDQEO-UHFFFAOYSA-N
Formula: C12H20N2O2
SMILES: O=C=NCCCCCCCCCN=C=O
Mol. weight [g/mol]: 224.30
CAS: 4538-39-0

Physical Properties

Property code	Value	Unit	Source
chs	-4458.90	kJ/mol	NIST Webbook
hf	-301.83	kJ/mol	Joback Method
hvap	61.37	kJ/mol	Joback Method
log10ws	-11.84		Crippen Method
logp	2.779		Crippen Method
mcvol	194.440	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
tb	607.30	K	Joback Method
tc	785.39	K	Joback Method

Sources

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=C4538390&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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