

2-Propanamine, N,N'-methanetetraylbis-

Other names:	Carbodiimide, diisopropyl- Diisopropylcarbodiimide N,N'-Diisopropylcarbodiimide N,N-Diisopropylcarbodiimide 1,3-Diisopropylcarbodiimide N,N'-methanetetraylbis(1-methylethylamine)
Inchi:	InChI=1S/C7H14N2/c1-6(2)8-5-9-7(3)4/h6-7H,1-4H3
InchiKey:	BDNKZNFMDZQMI-UHFFFAOYSA-N
Formula:	C7H14N2
SMILES:	CC(C)N=C=NC(C)C
Mol. weight [g/mol]:	126.20
CAS:	693-13-0

Physical Properties

Property code	Value	Unit	Source
chl	-4734.70	kJ/mol	NIST Webbook
hf	11.63	kJ/mol	Joback Method
hfl	-20.80	kJ/mol	NIST Webbook
hvap	37.50	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.977		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	908.00		NIST Webbook
tb	511.15	K	Joback Method
tc	728.75	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693130&Units=SI
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

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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