

3,3',3'',3''',3'''',3'''''-[(Cyclohexane-1,2,3,4,5,6-hexay

Inchi:

LnChI=1S/C24H30N6O6/c25-7-1-13-31-19-20(32-14-2-8-26)22(34-16-4-10-28)24(36-18-6

InchiKey:

LMHMIJYIOJVN MJ-UHFFFAOYSA-N

Formula:

C24H30N6O6

SMILES:

N#CCCOC1C(OCCC#N)C(OCCC#N)C(OCCC#N)C(OCCC#N)C1OCCC#N

Mol. weight [g/mol]:

498.53

Physical Properties

Property code	Value	Unit	Source
gf	306.18	kJ/mol	Joback Method
hf	-390.11	kJ/mol	Joback Method
hfus	71.27	kJ/mol	Joback Method
hvap	145.23	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	1.793		Crippen Method
mcvol	381.660	ml/mol	McGowan Method
pc	717.22	kPa	Joback Method
tb	1491.72	K	Joback Method
tc	1936.81	K	Joback Method
tf	869.74	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.74	J/mol×K	1491.72	Joback Method
cpg	1121.87	J/mol×K	1565.90	Joback Method
cpg	1049.88	J/mol×K	1640.08	Joback Method
cpg	963.20	J/mol×K	1714.27	Joback Method
cpg	861.29	J/mol×K	1788.45	Joback Method
cpg	743.61	J/mol×K	1862.63	Joback Method
cpg	609.60	J/mol×K	1936.81	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=B6009190&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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