Cyclododecylamine, n-methyl-

Inchi: InChI=1S/C13H27N/c1-14-13-11-9-7-5-3-2-4-6-8-10-12-13/h13-14H,2-12H2,1H3
InchiKey: DPKGRPBHAYLZKC-UHFFFAOYSA-N
Formula: C13H27N
SMILES: CNC1CCCCCCCCCCC1
Mol. weight [g/mol]: 197.36
CAS: 40221-53-2

Physical Properties

Property code	Value	Unit	Source
gf	99.82	kJ/mol	Joback Method
hf	-240.82	kJ/mol	Joback Method
hfus	13.76	kJ/mol	Joback Method
hvap	52.43	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.879		Crippen Method
mcvol	193.150	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
tb	592.18	K	Joback Method
tc	826.48	K	Joback Method
tf	275.19	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.70	J/mol×K	592.18	Joback Method
cpg	547.34	J/mol×K	631.23	Joback Method
cpg	573.25	J/mol×K	670.28	Joback Method
cpg	597.44	J/mol×K	709.33	Joback Method
cpg	619.90	J/mol×K	748.38	Joback Method
cpg	640.62	J/mol×K	787.43	Joback Method
cpg	659.59	J/mol×K	826.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40221532&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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