Cyclododecylamine

Other names:	Cyclododecanamine
Inchi:	InChI=1S/C12H25N/c13-12-10-8-6-4-2-1-3-5-7-9-11-12/h12H,1-11,13H2
InchiKey:	HBGGBCVEFUPUNY-UHFFFAOYSA-N
Formula:	C12H25N
SMILES:	NC1CCCCCCCCCCC1
Mol. weight [g/mol]:	183.33
CAS:	1502-03-0

Physical Properties

Property code	Value	Unit	Source
gf	68.46	kJ/mol	Joback Method
hf	-239.86	kJ/mol	Joback Method
hfus	11.27	kJ/mol	Joback Method
hvap	54.41	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.618		Crippen Method
mcvol	179.060	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
tb	591.66	K	Joback Method
tc	840.53	K	Joback Method
tf	294.52	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.75	J/mol×K	591.66	Joback Method
cpg	509.04	J/mol×K	633.14	Joback Method
cpg	534.51	J/mol×K	674.62	Joback Method
cpg	558.16	J/mol×K	716.10	Joback Method
cpg	579.97	J/mol×K	757.58	Joback Method
cpg	599.94	J/mol×K	799.05	Joback Method
cpg	618.05	J/mol×K	840.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.20	K	0.90	NIST Webbook

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=C1502030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with secondary, tertiary, and cyclic amines at 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.04.017

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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