

1,4,8,11-Tetraazacyclotetradecane

Other names:	Cyclam
Inchi:	InChI=1S/C10H24N4/c1-3-11-7-9-13-5-2-6-14-10-8-12-4-1/h11-14H,1-10H2
InchiKey:	MDAXKAUIABOHTD-UHFFFAOYSA-N
Formula:	C10H24N4
SMILES:	C1CNCCNCCCNCNC1
Mol. weight [g/mol]:	200.32
CAS:	295-37-4

Physical Properties

Property code	Value	Unit	Source
chs	-7249.00 ± 2.00	kJ/mol	NIST Webbook
gf	319.52	kJ/mol	Joback Method
hf	-73.11	kJ/mol	Joback Method
hfs	-116.00 ± 2.00	kJ/mol	NIST Webbook
hfus	33.98	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-0.66		Crippen Method
logp	-0.861		Crippen Method
mcvol	180.820	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	680.78	K	Joback Method
tc	962.13	K	Joback Method
tf	606.04	K	Joback Method
vc	0.614	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.13	J/mol×K	868.35	Joback Method
cpg	629.91	J/mol×K	915.24	Joback Method
cpg	519.71	J/mol×K	680.78	Joback Method
cpg	546.73	J/mol×K	727.67	Joback Method

cpg	571.40	J/mol×K	774.56	Joback Method
cpg	593.58	J/mol×K	821.45	Joback Method
cpg	643.78	J/mol×K	962.13	Joback Method
cps	374.61	J/mol×K	298.15	NIST Webbook
hsubt	133.90 ± 2.50	kJ/mol	362.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C295374&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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