Cypenamine

Inchi: InChI=1S/C11H15N/c12-11-8-4-7-10(11)9-5-2-1-3-6-9/h1-3,5-6,10-11H,4,7-8,12H2
InchiKey: VNGYTYNUZHDMPP-UHFFFAOYSA-N
Formula: C11H15N
SMILES: NC1CCCC1c1ccccc1
Mol. weight [g/mol]: 161.24
CAS: 5588-23-8

Physical Properties

Property code	Value	Unit	Source
gf	249.44	kJ/mol	Joback Method
hf	40.09	kJ/mol	Joback Method
hfus	18.49	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.281		Crippen Method
mcvol	141.210	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
rinpol	1428.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1405.00		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	1976.00		NIST Webbook
ripol	2030.00		NIST Webbook
ripol	2022.00		NIST Webbook
ripol	2014.00		NIST Webbook
ripol	1966.00		NIST Webbook
tb	560.90	K	Joback Method
tc	806.64	K	Joback Method
tf	330.07	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.34	J/mol×K	560.90	Joback Method
cpg	370.52	J/mol×K	601.86	Joback Method
cpg	388.29	J/mol×K	642.81	Joback Method
cpg	404.73	J/mol×K	683.77	Joback Method
cpg	419.91	J/mol×K	724.73	Joback Method
cpg	433.88	J/mol×K	765.68	Joback Method
cpg	446.73	J/mol×K	806.64	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=C5588238&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume