Ethinamate

Other names:	Cyclohexanol, 1-ethynyl-, carbamate
	Ethinamat
	Valamin
	Valmid
	Valmidate
	Volamin
	1-Ethinylcyclohexyl carbamate
	1-Ethynylcyclohexanol carbamate
	1-Ethynylcyclohexyl carbamate
	Carbamic acid, 1-ethynylcyclohexyl ester
	Etinamate
	USAF EL-42
	Valamina
	Valaminettae
	Valaminetten
	Aethinyl-cyclohexyl-carbamat
	Carbamate de l'ethinylcyclohexanol
	Ethinimate
	Cyclohexanol, 1-ethynyl-, 1-carbamate
	NSC 11538
Inchi:	InChI=1S/C9H13NO2/c1-2-9(12-8(10)11)6-4-3-5-7-9/h1H,3-7H2,(H2,10,11)
InchiKey:	GXRZIMHKGDIBEW-UHFFFAOYSA-N
Formula:	C9H13NO2
SMILES:	C#CC1(OC(N)=O)CCCCC1
Mol. weight [g/mol]:	167.21
CAS:	126-52-3

Physical Properties

Property code	Value	Unit	Source
gf	99.46	kJ/mol	Joback Method
hf	-78.64	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	54.56	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	1.418		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method

rinpol	1349.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1397.40		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1365.00		NIST Webbook
tb	564.05	K	Joback Method
tc	807.95	K	Joback Method
tf	424.86	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.24	J/mol×K	564.05	Joback Method
cpg	347.36	J/mol×K	604.70	Joback Method
cpg	361.42	J/mol×K	645.35	Joback Method
cpg	374.57	J/mol×K	686.00	Joback Method
cpg	386.97	J/mol×K	726.65	Joback Method
cpg	398.75	J/mol×K	767.30	Joback Method
cpg	410.08	J/mol×K	807.95	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=C126523&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume