

Cinnamylamine, n-methyl-n-2-propynyl-

Inchi:	InChI=1S/C13H15N/c1-3-11-14(2)12-7-10-13-8-5-4-6-9-13/h1,4-10H,11-12H2,2H3/b10-7
InchiKey:	NHDSFWYVAIGZBR-JXMROGBWSA-N
Formula:	C13H15N
SMILES:	C#CCN(C)CC=Cc1ccccc1
Mol. weight [g/mol]:	185.26
CAS:	125436-88-6

Physical Properties

Property code	Value	Unit	Source
gf	585.06	kJ/mol	Joback Method
hf	401.53	kJ/mol	Joback Method
hfus	29.67	kJ/mol	Joback Method
hvap	48.67	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.265		Crippen Method
mcvol	167.350	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
tb	530.24	K	Joback Method
tc	747.57	K	Joback Method
tf	337.05	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.21	J/molxK	530.24	Joback Method
cpg	389.91	J/molxK	566.46	Joback Method
cpg	405.43	J/molxK	602.68	Joback Method
cpg	419.87	J/molxK	638.90	Joback Method
cpg	433.30	J/molxK	675.12	Joback Method
cpg	445.80	J/molxK	711.35	Joback Method
cpg	457.44	J/molxK	747.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C125436886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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