Piperonylamine, n-methyl-n-2-propynyl-

Inchi: InChI=1S/C12H13NO2/c1-3-6-13(2)8-10-4-5-11-12(7-10)15-9-14-11/h1,4-5,7H,6,8-9H2,2
InchiKey: SGRNTWZMVNGHLS-UHFFFAOYSA-N
Formula: C12H13NO2
SMILES: C#CCN(C)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 203.24
CAS: 56862-18-1

Physical Properties

Property code	Value	Unit	Source
gf	373.38	kJ/mol	Joback Method
hf	111.15	kJ/mol	Joback Method
hfus	39.12	kJ/mol	Joback Method
hvap	57.05	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.480		Crippen Method
mcvol	158.440	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
tb	578.47	K	Joback Method
tc	803.96	K	Joback Method
tf	431.22	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.50	J/mol×K	578.47	Joback Method
cpg	404.00	J/mol×K	616.05	Joback Method
cpg	417.42	J/mol×K	653.63	Joback Method
cpg	429.87	J/mol×K	691.22	Joback Method
cpg	441.43	J/mol×K	728.80	Joback Method
cpg	452.18	J/mol×K	766.38	Joback Method
cpg	462.21	J/mol×K	803.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56862181&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

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