N-Methyl-di(2-propynyl)-amine

Other names: N,N-Di(2-propynyl)-N-methylamine
Inchi: InChI=1S/C7H9N/c1-4-6-8(3)7-5-2/h1-2H,6-7H2,3H3
InchiKey: SQRXWXCCRCQPKC-UHFFFAOYSA-N
Formula: C7H9N
SMILES: C#CCN(C)CC#C
Mol. weight [g/mol]: 107.15
CAS: 2568-61-8

Physical Properties

Property code	Value	Unit	Source
chl	-4507.00 ± 1.30	kJ/mol	NIST Webbook
gf	564.98	kJ/mol	Joback Method
hf	463.52	kJ/mol	Joback Method
hfl	466.00 ± 1.00	kJ/mol	NIST Webbook
hfus	22.86	kJ/mol	Joback Method
hvap	32.94	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	0.185		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	352.24	K	Joback Method
tc	539.13	K	Joback Method
tf	295.06	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.61	J/mol×K	352.24	Joback Method
cpg	185.73	J/mol×K	383.39	Joback Method
cpg	195.28	J/mol×K	414.54	Joback Method
cpg	204.28	J/mol×K	445.69	Joback Method
cpg	212.78	J/mol×K	476.83	Joback Method
cpg	220.78	J/mol×K	507.98	Joback Method

cpg	228.32	J/mol×K	539.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2568618&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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