Diethyl(1-propynyl)amine

Other names: N,N-diethyl-1-propynylamine
Inchi: InChI=1S/C7H13N/c1-4-7-8(5-2)6-3/h5-6H2,1-3H3
InchiKey: RJSCZBRDRBIRHP-UHFFFAOYSA-N
Formula: C7H13N
SMILES: CC#CN(CC)CC
Mol. weight [g/mol]: 111.18
CAS: 4231-35-0

Physical Properties

Property code	Value	Unit	Source
gf	321.64	kJ/mol	Joback Method
hf	152.02	kJ/mol	Joback Method
hfus	20.03	kJ/mol	Joback Method
hvap	35.37	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.309		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
tb	381.00	K	Joback Method
tc	567.59	K	Joback Method
tf	307.22	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.46	J/mol×K	381.00	Joback Method
cpg	210.44	J/mol×K	412.10	Joback Method
cpg	221.91	J/mol×K	443.20	Joback Method
cpg	232.87	J/mol×K	474.29	Joback Method
cpg	243.35	J/mol×K	505.39	Joback Method
cpg	253.35	J/mol×K	536.49	Joback Method

cpg	262.91	J/mol×K	567.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4231350&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume