2-Propenal, 3-(dimethylamino)-

Other names: «beta»-(Dimethylamino)acrolein
3-(Dimethylamino)acrolein
N,N-Dimethylamino-2-propen-3-al
3-(Dimethylamino)acrylaldehyde
3-(Dimethylamino)-2-propenal
Inchi: InChI=1S/C5H9NO/c1-6(2)4-3-5-7/h3-5H,1-2H3/b4-3+
InchiKey: RRLMPLDPCKRASL-ONEGZZNKSA-N
Formula: C5H9NO
SMILES: CN(C)C=CC=O
Mol. weight [g/mol]: 99.13
CAS: 927-63-9

Physical Properties

Property code	Value	Unit	Source
chl	-3079.00 ± 3.00	kJ/mol	NIST Webbook
gf	82.70	kJ/mol	Joback Method
hf	-104.00	kJ/mol	NIST Webbook
hfus	14.22	kJ/mol	Joback Method
hvap	71.00 ± 3.40	kJ/mol	NIST Webbook
log10ws	-0.11		Crippen Method
logp	0.261		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
tb	544.70	K	NIST Webbook
tc	559.78	K	Joback Method
tf	215.50	K	Joback Method
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.52	J/mol×K	379.06	Joback Method
cpg	164.96	J/mol×K	409.18	Joback Method
cpg	173.89	J/mol×K	439.30	Joback Method

cpg	182.35	J/mol×K	469.42	Joback Method
cpg	190.35	J/mol×K	499.54	Joback Method
cpg	197.91	J/mol×K	529.66	Joback Method
cpg	205.05	J/mol×K	559.78	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C927639&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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