

3-Dimethylaminoacrylonitrile

Other names:	3-(Dimethylamino)acrylonitrile,c&t 2-Propenenitrile, 3-(dimethylamino)- Dimethylaminoacrylonitril
Inchi:	InChI=1S/C5H8N2/c1-7(2)5-3-4-6/h3,5H,1-2H3
InchiKey:	ZKKBIZXAEDFPNL-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	CN(C)C=CC#N
Mol. weight [g/mol]:	96.13
CAS:	2407-68-3

Physical Properties

Property code	Value	Unit	Source
gf	315.40	kJ/mol	Joback Method
hf	203.10	kJ/mol	Joback Method
hfus	13.44	kJ/mol	Joback Method
hvap	39.20	kJ/mol	Joback Method
log10ws	-0.70		Crippen Method
logp	0.585		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	432.48	K	Joback Method
tc	630.66	K	Joback Method
tf	238.49	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.49	J/molxK	432.48	Joback Method
cpg	173.17	J/molxK	465.51	Joback Method
cpg	181.34	J/molxK	498.54	Joback Method
cpg	189.02	J/molxK	531.57	Joback Method
cpg	196.23	J/molxK	564.60	Joback Method
cpg	203.02	J/molxK	597.63	Joback Method

cpg

209.39

J/mol×K

630.66

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.20	K	0.04	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2407683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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