trans-dimethylamino acrylonitrile

Inchi: InChI=1S/C5H8N2/c1-7(2)5-3-4-6/h3,5H,1-2H3/b5-3+
InchiKey: ZKKBIZXAEDFPNL-HWKANZROSA-N
Formula: C5H8N2
SMILES: CN(C)C=CC#N
Mol. weight [g/mol]: 96.13
CAS: 35520-41-3

Physical Properties

Property code	Value	Unit	Source
affp	896.80	kJ/mol	NIST Webbook
basg	864.30	kJ/mol	NIST Webbook
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/mol×K	432.48	Joback Method
cpg	173.17	J/mol×K	465.51	Joback Method
cpg	181.34	J/mol×K	498.54	Joback Method
cpg	189.02	J/mol×K	531.57	Joback Method
cpg	196.23	J/mol×K	564.60	Joback Method
cpg	203.02	J/mol×K	597.63	Joback Method
cpg	209.39	J/mol×K	630.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35520413&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
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