Propanenitrile, 3,3',3''-nitrilotris-

Other names: Propionitrile, 3,3',3''-nitrilotri-
3,3',3''-Nitrilotripropionitrile
Amine, tris(2-cyanoethyl)-
Inchi: InChI=1S/C9H12N4/c10-4-1-7-13(8-2-5-11)9-3-6-12/h1-3,7-9H2
InchiKey: FYYPYNRGACGNNN-UHFFFAOYSA-N
Formula: C9H12N4
SMILES: N#CCCN(CCC#N)CCC#N
Mol. weight [g/mol]: 176.22
CAS: 7528-78-1

Physical Properties

Property code	Value	Unit	Source
gf	535.22	kJ/mol	Joback Method
hf	333.08	kJ/mol	Joback Method
hfus	26.61	kJ/mol	Joback Method
hvap	69.11	kJ/mol	Joback Method
ie	10.40	eV	NIST Webbook
log10ws	-1.76		Crippen Method
logp	1.029		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
tb	724.00	K	Joback Method
tc	933.67	K	Joback Method
tf	418.63	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.86	J/mol×K	724.00	Joback Method
cpg	402.80	J/mol×K	758.94	Joback Method
cpg	411.20	J/mol×K	793.89	Joback Method
cpg	419.08	J/mol×K	828.83	Joback Method
cpg	426.46	J/mol×K	863.78	Joback Method

cpg	433.39	J/mol×K	898.72	Joback Method
cpg	439.88	J/mol×K	933.67	Joback Method

Sources

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=C7528781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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