Propanenitrile, 3-(propylamino)-

Other names:	Propionitrile, 3-(propylamino)-
	N-(«beta»-Cyanoethyl)propylamine
	N-Cyanoethyl-N-propylamine
	3-(Propylamino)propionitrile
Inchi:	InChI=1S/C6H12N2/c1-2-5-8-6-3-4-7/h8H,2-3,5-6H2,1H3
InchiKey:	MZQXEAUWIMFFCG-UHFFFAOYSA-N
Formula:	C6H12N2
SMILES:	CCCNCCC#N
Mol. weight [g/mol]:	112.17
CAS:	7249-87-8

Physical Properties

Property code	Value	Unit	Source
gf	222.21	kJ/mol	Joback Method
hf	51.18	kJ/mol	Joback Method
hfus	17.90	kJ/mol	Joback Method
hvap	45.86	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.900		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	488.93	K	Joback Method
tc	680.58	K	Joback Method
tf	275.03	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.14	J/mol×K	488.93	Joback Method
cpg	240.07	J/mol×K	520.87	Joback Method
cpg	249.55	J/mol×K	552.81	Joback Method
cpg	258.59	J/mol×K	584.76	Joback Method
cpg	267.21	J/mol×K	616.70	Joback Method

cpg	275.42	J/mol×K	648.64	Joback Method
cpg	283.23	J/mol×K	680.58	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=C7249878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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