Propanenitrile, 3,3'-thiobis-

Other names:	Propionitrile, 3,3'-thiodi-
	«beta»,«beta»'-Dicyanodiethyl sulfide
	«beta»,«beta»'-Thiodipropionitrile
	Bis(2-cyanoethyl) sulfide
	Di(2-cyanoethyl) sulfide
	Dicyanoethyl sulfide
	Sulfide, bis(2-cyanoethyl)
	Thiodipropionitrile
	2-Cyanoethyl sulfide
	3,3'-Thiodipropionitrile
	Thiobis(2-cyanoethane)
	2-Cyanoethyl thioether
	Nitril kyseliny «beta»,«beta»'-thiodipropionove
	USAF HA-5
	2,2'-Thiodiethylkyanid
	Bis-(2-cyanoethyl) sulphide
	beta,beta'-Thiodipropionitrile
	NSC 2040
	3,3'-thiodipropiononitrile
Inchi:	InChI=1S/C6H8N2S/c7-3-1-5-9-6-2-4-8/h1-2,5-6H2
InchiKey:	NDVLTZFQVDXFAN-UHFFFAOYSA-N
Formula:	C6H8N2S
SMILES:	N#CCCSCCC#N
Mol. weight [g/mol]:	140.21
CAS:	111-97-7

Physical Properties

Property code	Value	Unit	Source
gf	299.12	kJ/mol	Joback Method
hf	204.46	kJ/mol	Joback Method
hfl	96.30 ± 5.00	kJ/mol	NIST Webbook
hfus	18.44	kJ/mol	Joback Method
hvap	56.72	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.547		Crippen Method
mcvol	114.510	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method

tb	609.62	K	Joback Method
tc	835.89	K	Joback Method
tf	295.25 ± 0.30	K	NIST Webbook
tf	301.75 ± 0.30	K	NIST Webbook
tf	301.70 ± 0.20	K	NIST Webbook
tf	301.80 ± 0.15	K	NIST Webbook
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.97	J/mol×K	609.62	Joback Method
cpg	255.88	J/mol×K	647.33	Joback Method
cpg	263.32	J/mol×K	685.04	Joback Method
cpg	270.32	J/mol×K	722.75	Joback Method
cpg	276.86	J/mol×K	760.47	Joback Method
cpg	282.97	J/mol×K	798.18	Joback Method
cpg	288.64	J/mol×K	835.89	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C111977&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

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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