Propanenitrile, 3,3'-oxybis-

Other names:	Propionitrile, 3,3'-oxydi-
	«beta»,«beta»'-Bis(cyanoethyl) ether
	«beta»,«beta»'-Dicyanodiethyl ether
	«beta»,«beta»'-Oxydipropionitrile
	Bis(2-cyanoethyl) ether
	3,3'-Oxydipropionitrile
	Bis(cyanoethyl)ether
	2-Cyanoethyl ether
	«beta», «beta»-oxydipropionitrile
	2,2'-Dicyanodiethyl ether
	di(2-Cyanoethyl)ether
	3,3-Oxydipropionitrile
	Ether, bis(2-cyanoethyl)
	2,2'-Oxydiethankarbonitril
	Bis(«beta»-Cyanoethyl) ether
	O(CH2CH2CN)2
	NSC 7769
	3,3'-oxydipropiononitrile
Inchi:	InChI=1S/C6H8N2O/c7-3-1-5-9-6-2-4-8/h1-2,5-6H2
InchiKey:	BCGCCTGNWPKXJL-UHFFFAOYSA-N
Formula:	C6H8N2O
SMILES:	N#CCCOCCC#N
Mol. weight [g/mol]:	124.14
CAS:	1656-48-0

Physical Properties

Property code	Value	Unit	Source
affp	813.80	kJ/mol	NIST Webbook
basg	786.40	kJ/mol	NIST Webbook
gf	161.00	kJ/mol	Joback Method
hf	30.37	kJ/mol	Joback Method
hfus	15.50	kJ/mol	Joback Method
hvap	52.32	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.830		Crippen Method
mcvol	104.030	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method

tb	563.26	K	Joback Method
tc	769.29	K	Joback Method
tf	246.85 ± 0.20	K	NIST Webbook
tf	246.77 ± 0.30	K	NIST Webbook
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.68	J/mol×K	563.26	Joback Method
cpg	236.32	J/mol×K	597.60	Joback Method
cpg	243.62	J/mol×K	631.94	Joback Method
cpg	250.59	J/mol×K	666.27	Joback Method
cpg	257.22	J/mol×K	700.61	Joback Method
cpg	263.50	J/mol×K	734.95	Joback Method
cpg	269.44	J/mol×K	769.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.20	K	0.07	NIST Webbook
tbrp	460.00 ± 1.00	K	2.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1656480&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

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