

2,2',2''-Nitrilotriethanol, methyl ether

Other names:	2,2'-[(2-Methoxyethyl)azanediyl]diethanol
Inchi:	InChI=1S/C7H17NO3/c1-11-7-4-8(2-5-9)3-6-10/h9-10H,2-7H2,1H3
InchiKey:	LANTZOPUEMHZGG-UHFFFAOYSA-N
Formula:	C7H17NO3
SMILES:	COCCN(CCO)CCO
Mol. weight [g/mol]:	163.21

Physical Properties

Property code	Value	Unit	Source
gf	-259.80	kJ/mol	Joback Method
hf	-556.96	kJ/mol	Joback Method
hfus	26.27	kJ/mol	Joback Method
hvap	68.99	kJ/mol	Joback Method
log10ws	1.06		Crippen Method
logp	-1.081		Crippen Method
mcvol	137.080	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1337.00		NIST Webbook
tb	578.78	K	Joback Method
tc	735.57	K	Joback Method
tf	344.99	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.42	J/mol×K	578.78	Joback Method
cpg	367.33	J/mol×K	604.91	Joback Method
cpg	376.85	J/mol×K	631.04	Joback Method
cpg	385.98	J/mol×K	657.18	Joback Method
cpg	394.75	J/mol×K	683.31	Joback Method
cpg	403.15	J/mol×K	709.44	Joback Method
cpg	411.20	J/mol×K	735.57	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=U378697&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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