4,4-Dimethoxybutyronitrile

Other names:	«beta»-Cyanopropionaldehyde dimethylacetal
	Butanenitrile, 4,4-dimethoxy-
	Cyanopropionaldehyde dimethyl acetal
	3-Cyanopropionaldehyde dimethyl acetal
Inchi:	InChI=1S/C6H11NO2/c1-8-6(9-2)4-3-5-7/h6H,3-4H2,1-2H3
InchiKey:	XJHNCGVHPLDMRK-UHFFFAOYSA-N
Formula:	C6H11NO2
SMILES:	COC(CCC#N)OC
Mol. weight [g/mol]:	129.16
CAS:	14618-78-1

Physical Properties

Property code	Value	Unit	Source
gf	-79.62	kJ/mol	Joback Method
hf	-272.01	kJ/mol	Joback Method
hfus	11.65	kJ/mol	Joback Method
hvap	43.86	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.909		Crippen Method
mcvol	108.520	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1020.00		NIST Webbook
tb	483.16	K	Joback Method
tc	674.45	K	Joback Method
tf	251.83	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.62	J/mol×K	483.16	Joback Method
cpg	241.98	J/mol×K	515.04	Joback Method
cpg	251.05	J/mol×K	546.92	Joback Method
cpg	259.82	J/mol×K	578.80	Joback Method

cpg	268.29	J/mol×K	610.68	Joback Method
cpg	276.45	J/mol×K	642.56	Joback Method
cpg	284.27	J/mol×K	674.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14618781&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume