Butanenitrile, 4,4-diethoxy-

Other names:	3-Cyanopropionaldehyde diethyl acetal
	Propionaldehyde, 3-cyano-, diethyl acetal
	4,4-diethoxybutanenitrile
Inchi:	InChI=1S/C8H15NO2/c1-3-10-8(11-4-2)6-5-7-9/h8H,3-6H2,1-2H3
InchiKey:	DRZCPHGVEATLFR-UHFFFAOYSA-N
Formula:	C8H15NO2
SMILES:	CCOC(CCC#N)OCC
Mol. weight [g/mol]:	157.21
CAS:	18381-45-8

Physical Properties

Property code	Value	Unit	Source
gf	-62.78	kJ/mol	Joback Method
hf	-313.29	kJ/mol	Joback Method
hfus	16.84	kJ/mol	Joback Method
hvap	48.31	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.689		Crippen Method
mcvol	136.700	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
tb	528.92	K	Joback Method
tc	715.81	K	Joback Method
tf	274.37	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.72	J/mol×K	528.92	Joback Method
cpg	329.35	J/mol×K	560.07	Joback Method
cpg	340.56	J/mol×K	591.22	Joback Method
cpg	351.34	J/mol×K	622.37	Joback Method
cpg	361.70	J/mol×K	653.51	Joback Method
cpg	371.61	J/mol×K	684.66	Joback Method

cpg	381.09	J/mol×K	715.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	1.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18381458&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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