

Acetaldehyde, di-sec-butyl acetal

Other names:	Ethane, 1,1-di-sec-butoxy-
Inchi:	InChI=1S/C10H22O2/c1-6-8(3)11-10(5)12-9(4)7-2/h8-10H,6-7H2,1-5H3
InchiKey:	CUOLYDYUVYAZFH-UHFFFAOYSA-N
Formula:	C10H22O2
SMILES:	CCC(C)OC(C)OC(C)CC
Mol. weight [g/mol]:	174.28
CAS:	5314-41-0

Physical Properties

Property code	Value	Unit	Source
gf	-184.00	kJ/mol	Joback Method
hf	-530.01	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	41.51	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.963		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
tb	444.00 ± 4.00	K	NIST Webbook
tc	644.52	K	Joback Method
tf	201.92	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.61	J/molxK	471.72	Joback Method
cpg	385.27	J/molxK	500.52	Joback Method
cpg	400.40	J/molxK	529.32	Joback Method
cpg	415.02	J/molxK	558.12	Joback Method
cpg	429.12	J/molxK	586.92	Joback Method
cpg	442.70	J/molxK	615.72	Joback Method
cpg	455.76	J/molxK	644.52	Joback Method
dvisc	0.0139337	Paxs	201.92	Joback Method

dvisc	0.0032621	Paxs	246.89	Joback Method
dvisc	0.0011946	Paxs	291.85	Joback Method
dvisc	0.0005721	Paxs	336.82	Joback Method
dvisc	0.0003258	Paxs	381.79	Joback Method
dvisc	0.0002090	Paxs	426.75	Joback Method
dvisc	0.0001458	Paxs	471.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5314410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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