

Acetaldehyde ethyleneglycol acetal 1

Other names:	1,3-Dioxolane, 2-methyl-4-phenyl, # 2
Inchi:	InChI=1S/C10H12O2/c1-8-11-7-10(12-8)9-5-3-2-4-6-9/h2-6,8,10H,7H2,1H3
InchiKey:	YPPGSWWESBCSCT-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC1OCC(c2ccccc2)O1
Mol. weight [g/mol]:	164.20

Physical Properties

Property code	Value	Unit	Source
gf	2.33	kJ/mol	Joback Method
hf	-237.06	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.120		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	1333.00		NIST Webbook
rinpol	1333.00		NIST Webbook
ripol	1793.00		NIST Webbook
ripol	1793.00		NIST Webbook
tb	519.39	K	Joback Method
tc	755.09	K	Joback Method
tf	288.68	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.09	J/molxK	519.39	Joback Method
cpg	320.49	J/molxK	558.67	Joback Method
cpg	336.71	J/molxK	597.96	Joback Method
cpg	351.79	J/molxK	637.24	Joback Method
cpg	365.79	J/molxK	676.52	Joback Method

cpg	378.75	J/molxK	715.81	Joback Method
cpg	390.71	J/molxK	755.09	Joback Method
dvisc	0.0031452	Paxs	288.68	Joback Method
dvisc	0.0017769	Paxs	327.13	Joback Method
dvisc	0.0011320	Paxs	365.58	Joback Method
dvisc	0.0007857	Paxs	404.04	Joback Method
dvisc	0.0005811	Paxs	442.49	Joback Method
dvisc	0.0004511	Paxs	480.94	Joback Method
dvisc	0.0003635	Paxs	519.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U284904&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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