alpha,alpha-OXYDIACETIC ACID

Other names:	Acetic acid, 2,2'-oxybis-
	Acetic acid, oxydi-
	Bis(carboxymethyl)ether
	Oxodiacetic acid
	Oxydiacetic acid
	Oxydiethanolic acid
	3-Oxapentanedioic acid
	Oxybisacetic acid
	2,2'-Oxydiacetic acid
	«alpha»,«alpha»-Oxydiacetic acid
	Anhydroglycolic acid
	NSC 8651
	3-Oxapentane-1,5-dioic acid
Inchi:	InChI=1S/C4H6O5/c5-3(6)1-9-2-4(7)8/h1-2H2,(H,5,6)(H,7,8)
InchiKey:	QEVGZEDELICMKH-UHFFFAOYSA-N
Formula:	C4H6O5
SMILES:	O=C(O)COCC(=O)O
Mol. weight [g/mol]:	134.09

Physical Properties

Property code	Value	Unit	Source
hfus	18.68	kJ/mol	Joback Method
hvap	89.77	kJ/mol	Cheméo Relay (1.0)
ie	9.90	eV	Cheméo Relay (1.0)
log10ws	0.59		Cheméo Relay (1.0)
logp	-0.828		Crippen Method
mcvol	87.970	ml/mol	McGowan Method
pc	5836.07	kPa	Joback Method
tb	523.50	K	Cheméo Relay (1.0)
tf	415.35	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	208.75	J/mol×K	605.44	Joback Method
cpg	214.05	J/mol×K	634.68	Joback Method
cpg	219.12	J/mol×K	663.93	Joback Method
cpg	223.95	J/mol×K	693.17	Joback Method
cpg	228.54	J/mol×K	722.41	Joback Method
cpg	232.88	J/mol×K	751.65	Joback Method
cpg	236.98	J/mol×K	780.90	Joback Method
dvisc	0.0046134	Pa×s	378.57	Joback Method
dvisc	0.0014796	Pa×s	416.38	Joback Method
dvisc	0.0005735	Pa×s	454.19	Joback Method
dvisc	0.0002571	Pa×s	492.00	Joback Method
dvisc	0.0001293	Pa×s	529.82	Joback Method
dvisc	0.0000712	Pa×s	567.63	Joback Method
dvisc	0.0000423	Pa×s	605.44	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C110996&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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
tf: Normal melting (fusion) point