1,2,4-Trioxolane

Inchi: InChI=1S/C2H4O3/c1-3-2-5-4-1/h1-2H2
InchiKey: RZYIPLSVRHWROD-UHFFFAOYSA-N
Formula: C2H4O3
SMILES: C1OCOO1
Mol. weight [g/mol]: 76.05
CAS: 289-14-5

Physical Properties

Property code	Value	Unit	Source
gf	-349.97	kJ/mol	Joback Method
hf	-434.59	kJ/mol	Joback Method
hfus	12.45	kJ/mol	Joback Method
hvap	32.01	kJ/mol	Joback Method
ie	10.67 ± 0.03	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
log10ws	0.20		Crippen Method
logp	-0.120		Crippen Method
mcvol	45.790	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
tb	337.47	K	Joback Method
tc	523.28	K	Joback Method
tf	206.90	K	Joback Method
vc	0.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	94.95	J/mol×K	523.28	Joback Method
cpg	91.84	J/mol×K	492.31	Joback Method
cpg	88.45	J/mol×K	461.34	Joback Method
cpg	84.77	J/mol×K	430.37	Joback Method
cpg	80.77	J/mol×K	399.41	Joback Method
cpg	76.44	J/mol×K	368.44	Joback Method
cpg	71.75	J/mol×K	337.47	Joback Method

dvisc	0.0014676	Pa×s	206.90	Joback Method
dvisc	0.0004486	Pa×s	337.47	Joback Method
dvisc	0.0005106	Pa×s	315.71	Joback Method
dvisc	0.0005924	Pa×s	293.95	Joback Method
dvisc	0.0007039	Pa×s	272.19	Joback Method
dvisc	0.0008617	Pa×s	250.42	Joback Method
dvisc	0.0010964	Pa×s	228.66	Joback Method
hvapt	34.80	kJ/mol	281.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C289145&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
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
hvapt: Enthalpy of vaporization at a given temperature
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume