Methylene glycol monoacetate

Other names: Methylene glycol monoacetate
Inchi: InChI=1S/C3H6O3/c1-3(5)6-2-4/h4H,2H2,1H3
InchiKey: JYVNDCLJHKQUHE-UHFFFAOYSA-N
Formula: C3H6O3
SMILES: CC(=O)OCO
Mol. weight [g/mol]: 90.08

Physical Properties

Property code	Value	Unit	Source
af	0.6125		Cheméo Relay (1.0)
gf	-396.36	kJ/mol	Joback Method
hf	-604.02	kJ/mol	Cheméo Relay (1.0)
hfus	10.40	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Cheméo Relay (1.0)
ie	10.27	eV	Cheméo Relay (1.0)
log10ws	0.83		Cheméo Relay (1.0)
logp	-0.501		Crippen Method
mcvol	66.440	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
tb	407.76	K	Cheméo Relay (1.0)
tc	619.60	K	Cheméo Relay (1.0)
tf	206.46	K	Cheméo Relay (1.0)
vc	0.245	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.32	J/mol×K	436.51	Joback Method
cpg	158.17	J/mol×K	611.34	Joback Method
cpg	153.74	J/mol×K	582.20	Joback Method
cpg	149.15	J/mol×K	553.06	Joback Method
cpg	144.41	J/mol×K	523.92	Joback Method
cpg	139.52	J/mol×K	494.79	Joback Method
cpg	134.49	J/mol×K	465.65	Joback Method

cpl	214.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0012605	Pa×s	346.53	Joback Method
dvisc	0.0002559	Pa×s	436.51	Joback Method
dvisc	0.0004025	Pa×s	406.52	Joback Method
dvisc	0.0006806	Pa×s	376.52	Joback Method
dvisc	0.0190072	Pa×s	256.55	Joback Method
dvisc	0.0026236	Pa×s	316.54	Joback Method
dvisc	0.0063665	Pa×s	286.54	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86011338&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

af: Acentric Factor
cpg: Ideal gas heat capacity
cpl: Liquid phase 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
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