DIETHYL 3-HYDROXYGLUTARATE

Other names: Diethyl- «beta»-hydroxyglutarate
Pentanedioic acid, 3-hydroxy-, diethyl ester
Inchi: InChI=1S/C9H16O5/c1-3-13-8(11)5-7(10)6-9(12)14-4-2/h7,10H,3-6H2,1-2H3
InchiKey: OLLQYIBTJXUEEX-UHFFFAOYSA-N
Formula: C9H16O5
SMILES: CCOC(=O)CC(O)CC(=O)OCC
Mol. weight [g/mol]: 204.22

Physical Properties

Property code	Value	Unit	Source
af	0.7778		Cheméo Relay (1.0)
gf	-582.20	kJ/mol	Joback Method
hf	-1066.06	kJ/mol	Cheméo Relay (1.0)
hfus	25.21	kJ/mol	Joback Method
hvap	75.76	kJ/mol	Cheméo Relay (1.0)
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-0.38		Cheméo Relay (1.0)
logp	0.254		Crippen Method
mcvol	158.420	ml/mol	McGowan Method
pc	2799.47	kPa	Joback Method
tb	523.91	K	Cheméo Relay (1.0)
tc	708.55	K	Cheméo Relay (1.0)
tf	292.27	K	Cheméo Relay (1.0)
vc	0.605	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.95	J/mol×K	649.64	Joback Method
cpg	432.85	J/mol×K	679.31	Joback Method
cpg	443.26	J/mol×K	708.98	Joback Method
cpg	453.15	J/mol×K	738.65	Joback Method
cpg	462.54	J/mol×K	768.32	Joback Method
cpg	471.41	J/mol×K	797.99	Joback Method

cpg	479.77	J/mol×K	827.66	Joback Method
dvisc	0.0027887	Pa×s	381.33	Joback Method
dvisc	0.0010206	Pa×s	426.05	Joback Method
dvisc	0.0004521	Pa×s	470.77	Joback Method
dvisc	0.0002307	Pa×s	515.49	Joback Method
dvisc	0.0001310	Pa×s	560.20	Joback Method
dvisc	0.0000809	Pa×s	604.92	Joback Method
dvisc	0.0000534	Pa×s	649.64	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.70	K	3.10	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32328033&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

Legend

af: Acentric Factor
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume