HEXANEDIOIC ACID, 3-OXO-, DIMETHYL ESTER

Other names: Hexanedioic acid, 3-oxo-, dimethyl ester
3-Oxohexanedioic acid, dimethyl ester
Inchi: InChI=1S/C8H12O5/c1-12-7(10)4-3-6(9)5-8(11)13-2/h3-5H2,1-2H3
InchiKey: CMGTZMRSJJKAPM-UHFFFAOYSA-N
Formula: C8H12O5
SMILES: COC(=O)CCC(=O)CC(=O)OC
Mol. weight [g/mol]: 188.18

Physical Properties

Property code	Value	Unit	Source
af	0.6172		Cheméo Relay (1.0)
hf	-922.30	kJ/mol	Cheméo Relay (1.0)
hfus	23.65	kJ/mol	Joback Method
hvap	71.37	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-0.62		Cheméo Relay (1.0)
logp	0.072		Crippen Method
mcvol	140.030	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
tb	515.82	K	Cheméo Relay (1.0)
tc	695.87	K	Cheméo Relay (1.0)
tf	306.75	K	Cheméo Relay (1.0)
vc	0.519	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.61	J/mol×K	588.89	Joback Method
cpg	394.43	J/mol×K	780.70	Joback Method
cpg	386.22	J/mol×K	748.74	Joback Method
cpg	377.48	J/mol×K	716.77	Joback Method
cpg	368.25	J/mol×K	684.80	Joback Method
cpg	358.52	J/mol×K	652.83	Joback Method
cpg	348.30	J/mol×K	620.86	Joback Method

dvisc	0.0005148	Pa×s	481.53	Joback Method
dvisc	0.0002372	Pa×s	588.89	Joback Method
dvisc	0.0002970	Pa×s	553.10	Joback Method
dvisc	0.0003837	Pa×s	517.32	Joback Method
dvisc	0.0017428	Pa×s	374.17	Joback Method
dvisc	0.0007242	Pa×s	445.74	Joback Method
dvisc	0.0010812	Pa×s	409.96	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5457443&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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