4-Oxoheptanedioic acid, diethyl ester

Other names:	Diethyl «gamma»-ketopimelate
	Heptanedioic acid, 4-oxo-, diethyl ester
	4-Oxoheptanedioic acid, diethyl ester
	diethyl 4-oxoheptanedioate
Inchi:	InChI=1S/C11H18O5/c1-3-15-10(13)7-5-9(12)6-8-11(14)16-4-2/h3-8H2,1-2H3
InchiKey:	ZGBUXZJMZBBISR-UHFFFAOYSA-N
Formula:	C11H18O5
SMILES:	CCOC(=O)CCC(=O)CCC(=O)OCC
Mol. weight [g/mol]:	230.26

Physical Properties

Property code	Value	Unit	Source
af	0.7154		Cheméo Relay (1.0)
gf	-555.02	kJ/mol	Joback Method
hf	-1022.52	kJ/mol	Cheméo Relay (1.0)
hfus	31.42	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Cheméo Relay (1.0)
ie	9.36	eV	Cheméo Relay (1.0)
log10ws	-1.08		Cheméo Relay (1.0)
logp	1.242		Crippen Method
mcvol	182.300	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
tb	550.13	K	Cheméo Relay (1.0)
tc	712.79	K	Cheméo Relay (1.0)
tf	314.79	K	Cheméo Relay (1.0)
vc	0.690	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.24	J/mol×K	657.53	Joback Method
cpg	497.14	J/mol×K	688.54	Joback Method
cpg	509.41	J/mol×K	719.55	Joback Method
cpg	521.04	J/mol×K	750.56	Joback Method

cpg	532.02	J/mol×K	781.57	Joback Method
cpg	542.36	J/mol×K	812.58	Joback Method
cpg	552.05	J/mol×K	843.59	Joback Method
dvisc	0.0014910	Pa×s	407.98	Joback Method
dvisc	0.0008793	Pa×s	449.57	Joback Method
dvisc	0.0005670	Pa×s	491.16	Joback Method
dvisc	0.0003916	Pa×s	532.75	Joback Method
dvisc	0.0002853	Pa×s	574.35	Joback Method
dvisc	0.0002170	Pa×s	615.94	Joback Method
dvisc	0.0001708	Pa×s	657.53	Joback Method

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=C6317493&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
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume