Diethyl 4-oxopimelate

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
CAS:	6317-49-3

Physical Properties

Property code	Value	Unit	Source
gf	-555.02	kJ/mol	Joback Method
hf	-872.55	kJ/mol	Joback Method
hfus	31.42	kJ/mol	Joback Method
hvap	65.14	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.242		Crippen Method
mcvol	182.300	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
tb	657.53	K	Joback Method
tc	843.59	K	Joback Method
tf	407.98	K	Joback Method
vc	0.706	m3/kmol	Joback Method

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:	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6317493&Units=SI

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
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

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