Diethyl pimelate

Other names:	1,5-Pentanedicarboxylic acid diethyl ester
	Pimelic acid diethyl ester
	Heptanedioic acid, diethyl ester
Inchi:	InChI=1S/C11H20O4/c1-3-14-10(12)8-6-5-7-9-11(13)15-4-2/h3-9H2,1-2H3
InchiKey:	LKKOGZVQGQUVHF-UHFFFAOYSA-N
Formula:	C11H20O4
SMILES:	CCOC(=O)CCCCCC(=O)OCC
Mol. weight [g/mol]:	216.27
CAS:	2050-20-6

Physical Properties

Property code	Value	Unit	Source
gf	-426.10	kJ/mol	Joback Method
hf	-759.97	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	58.39	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.063		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1480.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1453.00		NIST Webbook
tb	603.66	K	Joback Method
tc	782.25	K	Joback Method
tf	252.80 ± 0.60	K	NIST Webbook
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.03	J/mol×K	603.66	Joback Method
cpg	478.94	J/mol×K	633.43	Joback Method
cpg	492.26	J/mol×K	663.19	Joback Method

cpg	505.00	J/mol×K	692.96	Joback Method
cpg	517.15	J/mol×K	722.72	Joback Method
cpg	528.71	J/mol×K	752.49	Joback Method
cpg	539.69	J/mol×K	782.25	Joback Method
dvisc	0.0018153	Pa×s	358.05	Joback Method
dvisc	0.0009995	Pa×s	398.99	Joback Method
dvisc	0.0006149	Pa×s	439.92	Joback Method
dvisc	0.0004109	Pa×s	480.86	Joback Method
dvisc	0.0002926	Pa×s	521.79	Joback Method
dvisc	0.0002188	Pa×s	562.73	Joback Method
dvisc	0.0001703	Pa×s	603.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	466.20	K	13.30	NIST Webbook

Sources

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=C2050206&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume