Pimelic acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C23H44O4/c1-18(14-22(3,4)5)16-26-20(24)12-10-9-11-13-21(25)27-17-19(2)15
InchiKey: ZPRXJYHZQIEPII-UHFFFAOYSA-N
Formula: C23H44O4
SMILES: CC(COC(=O)CCCCCC(=O)OCC(C)CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-324.26	kJ/mol	Joback Method
hf	-1035.71	kJ/mol	Joback Method
hfus	39.03	kJ/mol	Joback Method
hvap	81.74	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	6.168		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	929.51	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	870.88	K	Joback Method
tc	1068.71	K	Joback Method
tf	468.13	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.01	J/mol×K	870.88	Joback Method
cpg	1175.35	J/mol×K	903.85	Joback Method
cpg	1193.47	J/mol×K	936.82	Joback Method
cpg	1210.42	J/mol×K	969.80	Joback Method
cpg	1226.26	J/mol×K	1002.77	Joback Method
cpg	1241.05	J/mol×K	1035.74	Joback Method
cpg	1254.84	J/mol×K	1068.71	Joback Method
dvisc	0.0007283	Pa×s	468.13	Joback Method

dvisc	0.0002653	Pa×s	535.25	Joback Method
dvisc	0.0001211	Pa×s	602.38	Joback Method
dvisc	0.0000646	Pa×s	669.50	Joback Method
dvisc	0.0000387	Pa×s	736.63	Joback Method
dvisc	0.0000252	Pa×s	803.75	Joback Method
dvisc	0.0000176	Pa×s	870.88	Joback Method

Sources

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=U406487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume