Trimellitic acid, 2,2,4-trimethylpentyl ester

Inchi: InChI=1S/C33H54O6/c1-22(2)16-31(7,8)19-37-28(34)25-13-14-26(29(35)38-20-32(9,10)
InchiKey: GFNQLDIWJXUYKC-UHFFFAOYSA-N
Formula: C33H54O6
SMILES: CC(C)CC(C)(C)COC(=O)c1ccc(C(=O)OCC(C)(C)CC(C)C)c(C(=O)OCC(C)(C)CC(C)C)c1
Mol. weight [g/mol]: 546.78
CAS: 53046-84-7

Physical Properties

Property code	Value	Unit	Source
gf	-380.43	kJ/mol	Joback Method
hf	-1287.35	kJ/mol	Joback Method
hfus	50.04	kJ/mol	Joback Method
hvap	115.07	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.374		Crippen Method
mcvol	474.390	ml/mol	McGowan Method
pc	669.08	kPa	Joback Method
tb	1208.94	K	Joback Method
tc	1498.91	K	Joback Method
tf	691.87	K	Joback Method
vc	1.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1724.23	J/mol×K	1208.94	Joback Method
cpg	1740.94	J/mol×K	1257.27	Joback Method
cpg	1755.91	J/mol×K	1305.60	Joback Method
cpg	1769.40	J/mol×K	1353.93	Joback Method
cpg	1781.67	J/mol×K	1402.26	Joback Method
cpg	1792.97	J/mol×K	1450.58	Joback Method
cpg	1803.57	J/mol×K	1498.91	Joback Method
dvisc	0.0000382	Pa×s	691.87	Joback Method
dvisc	0.0000164	Pa×s	778.05	Joback Method

dvisc	0.0000083	Pa×s	864.23	Joback Method
dvisc	0.0000048	Pa×s	950.40	Joback Method
dvisc	0.0000030	Pa×s	1036.58	Joback Method
dvisc	0.0000020	Pa×s	1122.76	Joback Method
dvisc	0.0000015	Pa×s	1208.94	Joback Method

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=C53046847&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume