Phthalic acid, 2,4-dimethylpent-3-yl tetradecyl ester

Inchi: InChI=1S/C29H48O4/c1-6-7-8-9-10-11-12-13-14-15-16-19-22-32-28(30)25-20-17-18-21-

InchiKey: PLRMLBXUAOURDR-UHFFFAOYSA-N

Formula: C29H48O4

SMILES: CCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(C(C)C)C(C)C

Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-179.08	kJ/mol	Joback Method
hf	-922.27	kJ/mol	Joback Method
hfus	59.52	kJ/mol	Joback Method
hvap	100.23	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.382		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	784.63	kPa	Joback Method
rinpol	3106.00		NIST Webbook
rinpol	3106.00		NIST Webbook
tb	1045.84	K	Joback Method
tc	1284.97	K	Joback Method
tf	554.85	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.75	J/mol×K	1045.84	Joback Method
cpg	1505.64	J/mol×K	1245.12	Joback Method
cpg	1494.76	J/mol×K	1205.26	Joback Method
cpg	1482.20	J/mol×K	1165.41	Joback Method
cpg	1467.90	J/mol×K	1125.55	Joback Method
cpg	1451.78	J/mol×K	1085.70	Joback Method
cpg	1514.93	J/mol×K	1284.97	Joback Method
dvisc	0.0000107	Pa×s	1045.84	Joback Method

dvisc	0.0000147	Pa×s	964.01	Joback Method
dvisc	0.0000213	Pa×s	882.18	Joback Method
dvisc	0.0000334	Pa×s	800.35	Joback Method
dvisc	0.0000580	Pa×s	718.51	Joback Method
dvisc	0.0001159	Pa×s	636.68	Joback Method
dvisc	0.0002843	Pa×s	554.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356853&Units=SI
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

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