Isophthalic acid, 3,3-dimethylbut-2-yl pentadecyl ester

Inchi: InChI=1S/C29H48O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-22-32-27(30)25-20-19-21-

InchiKey: HGOGDLVEYRADDR-UHFFFAOYSA-N

Formula: C29H48O4

SMILES: CCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)(C)C)c1

Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-171.36	kJ/mol	Joback Method
hf	-920.46	kJ/mol	Joback Method
hfus	59.15	kJ/mol	Joback Method
hvap	99.71	kJ/mol	Joback Method
log10ws	-9.78		Crippen Method
logp	8.526		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	785.95	kPa	Joback Method
rinpol	3207.00		NIST Webbook
rinpol	3207.00		NIST Webbook
tb	1043.49	K	Joback Method
tc	1280.94	K	Joback Method
tf	587.27	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.20	J/mol×K	1043.49	Joback Method
cpg	1509.66	J/mol×K	1241.37	Joback Method
cpg	1497.27	J/mol×K	1201.79	Joback Method
cpg	1483.54	J/mol×K	1162.22	Joback Method
cpg	1468.35	J/mol×K	1122.64	Joback Method
cpg	1451.61	J/mol×K	1083.07	Joback Method
cpg	1520.81	J/mol×K	1280.94	Joback Method
dvisc	0.0000097	Pa×s	1043.49	Joback Method

dvisc	0.0000132	Pa×s	967.45	Joback Method
dvisc	0.0000188	Pa×s	891.42	Joback Method
dvisc	0.0000287	Pa×s	815.38	Joback Method
dvisc	0.0000477	Pa×s	739.34	Joback Method
dvisc	0.0000892	Pa×s	663.31	Joback Method
dvisc	0.0001963	Pa×s	587.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356560&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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