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

Inchi: InChI=1S/C30H50O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-33-28(31)26-21-20-

InchiKey: BVKKSXAFKWXPHY-UHFFFAOYSA-N

Formula: C30H50O4

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

Mol. weight [g/mol]: 474.72

Physical Properties

Property code	Value	Unit	Source
gf	-162.94	kJ/mol	Joback Method
hf	-941.10	kJ/mol	Joback Method
hfus	61.74	kJ/mol	Joback Method
hvap	101.94	kJ/mol	Joback Method
log10ws	-10.20		Crippen Method
logp	8.916		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	745.29	kPa	Joback Method
rinpol	3313.00		NIST Webbook
rinpol	3313.00		NIST Webbook
tb	1066.37	K	Joback Method
tc	1312.45	K	Joback Method
tf	598.54	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.02	J/mol×K	1066.37	Joback Method
cpg	1574.63	J/mol×K	1271.44	Joback Method
cpg	1562.16	J/mol×K	1230.42	Joback Method
cpg	1548.28	J/mol×K	1189.41	Joback Method
cpg	1532.87	J/mol×K	1148.40	Joback Method
cpg	1515.83	J/mol×K	1107.38	Joback Method
cpg	1585.83	J/mol×K	1312.45	Joback Method
dvisc	0.0000082	Pa×s	1066.37	Joback Method

dvisc	0.0000112	Pa×s	988.40	Joback Method
dvisc	0.0000160	Pa×s	910.43	Joback Method
dvisc	0.0000245	Pa×s	832.45	Joback Method
dvisc	0.0000409	Pa×s	754.48	Joback Method
dvisc	0.0000769	Pa×s	676.51	Joback Method
dvisc	0.0001704	Pa×s	598.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356561&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