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

Inchi: InChI=1S/C24H38O4/c1-6-7-8-9-10-11-12-13-17-27-22(25)20-15-14-16-21(18-20)23(26)28-19(2)24(3,4)5/h14-16,18-19H,6-13,17H2,1-5H3

InchiKey: PUMSPAVLFXGOFB-UHFFFAOYSA-N

Formula: C24H38O4

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

Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-213.46	kJ/mol	Joback Method
hf	-817.26	kJ/mol	Joback Method
hfus	46.20	kJ/mol	Joback Method
hvap	88.58	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.575		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook
tb	929.09	K	Joback Method
tc	1140.66	K	Joback Method
tf	530.92	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.03	J/mol×K	929.09	Joback Method
cpg	1192.72	J/mol×K	1105.40	Joback Method
cpg	1180.59	J/mol×K	1070.14	Joback Method
cpg	1167.30	J/mol×K	1034.87	Joback Method
cpg	1152.82	J/mol×K	999.61	Joback Method
cpg	1137.08	J/mol×K	964.35	Joback Method
cpg	1203.78	J/mol×K	1140.66	Joback Method
dvisc	0.0000216	Pa×s	929.09	Joback Method

dvisc	0.0000290	Pa×s	862.73	Joback Method
dvisc	0.0000410	Pa×s	796.37	Joback Method
dvisc	0.0000616	Pa×s	730.00	Joback Method
dvisc	0.0001003	Pa×s	663.64	Joback Method
dvisc	0.0001823	Pa×s	597.28	Joback Method
dvisc	0.0003846	Pa×s	530.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356555&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