Isophthalic acid, 4-methylpent-2-yl tetradecyl ester

Inchi: InChI=1S/C28H46O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-20-31-27(29)25-18-17-19-26(2

InchiKey: LCOVGWLTLNJMEV-UHFFFAOYSA-N

Formula: C28H46O4

SMILES: CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CC(C)C)c1

Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-185.06	kJ/mol	Joback Method
hf	-896.35	kJ/mol	Joback Method
hfus	60.46	kJ/mol	Joback Method
hvap	98.40	kJ/mol	Joback Method
log10ws	-9.36		Crippen Method
logp	8.136		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	824.79	kPa	Joback Method
rinpol	3105.00		NIST Webbook
tb	1023.40	K	Joback Method
tc	1255.68	K	Joback Method
tf	558.58	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.15	J/mol×K	1023.40	Joback Method
cpg	1442.65	J/mol×K	1216.97	Joback Method
cpg	1431.44	J/mol×K	1178.25	Joback Method
cpg	1418.64	J/mol×K	1139.54	Joback Method
cpg	1404.21	J/mol×K	1100.83	Joback Method
cpg	1388.07	J/mol×K	1062.11	Joback Method
cpg	1452.37	J/mol×K	1255.68	Joback Method
dvisc	0.0000138	Pa×s	1023.40	Joback Method
dvisc	0.0000187	Pa×s	945.93	Joback Method

dvisc	0.0000266	Pa×s	868.46	Joback Method
dvisc	0.0000405	Pa×s	790.99	Joback Method
dvisc	0.0000677	Pa×s	713.52	Joback Method
dvisc	0.0001282	Pa×s	636.05	Joback Method
dvisc	0.0002898	Pa×s	558.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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