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

Inchi: InChI=1S/C27H44O4/c1-6-7-8-9-10-11-12-13-14-17-20-30-26(28)23-18-15-16-19-24(23)27(29)31-25(21(2)3)22(4)5/h15-16,18-19,21-22,25H,6-14,17,20H2,1-5H3

InchiKey: SKVWVZAAEKKUJI-UHFFFAOYSA-N

Formula: C27H44O4

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

Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-195.92	kJ/mol	Joback Method
hf	-880.99	kJ/mol	Joback Method
hfus	54.34	kJ/mol	Joback Method
hvap	95.78	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.602		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	876.36	kPa	Joback Method
rinpol	2901.00		NIST Webbook
rinpol	2901.00		NIST Webbook
tb	1000.08	K	Joback Method
tc	1224.77	K	Joback Method
tf	532.31	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.41	J/mol×K	1000.08	Joback Method
cpg	1324.96	J/mol×K	1037.53	Joback Method
cpg	1340.85	J/mol×K	1074.98	Joback Method
cpg	1355.13	J/mol×K	1112.42	Joback Method
cpg	1367.86	J/mol×K	1149.87	Joback Method
cpg	1379.09	J/mol×K	1187.32	Joback Method
cpg	1388.88	J/mol×K	1224.77	Joback Method
dvisc	0.0003750	Pa×s	532.31	Joback Method

dvisc	0.0001549	Pa×s	610.27	Joback Method
dvisc	0.0000781	Pa×s	688.23	Joback Method
dvisc	0.0000453	Pa×s	766.19	Joback Method
dvisc	0.0000291	Pa×s	844.16	Joback Method
dvisc	0.0000201	Pa×s	922.12	Joback Method
dvisc	0.0000147	Pa×s	1000.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356851&Units=SI

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