Terephthalic acid, dodecyl 5-methylhex-2-yl ester

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

InchiKey: NSSNDIXCGZMWLQ-UHFFFAOYSA-N

Formula: C27H44O4

SMILES: CCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(C)CCC(C)C)cc1

Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-193.48	kJ/mol	Joback Method
hf	-875.71	kJ/mol	Joback Method
hfus	57.87	kJ/mol	Joback Method
hvap	96.17	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.746		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	872.22	kPa	Joback Method
rinpol	3467.00		NIST Webbook
rinpol	3467.00		NIST Webbook
tb	1000.52	K	Joback Method
tc	1225.74	K	Joback Method
tf	547.31	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.09	J/mol×K	1000.52	Joback Method
cpg	1324.74	J/mol×K	1038.06	Joback Method
cpg	1340.74	J/mol×K	1075.59	Joback Method
cpg	1355.13	J/mol×K	1113.13	Joback Method
cpg	1367.98	J/mol×K	1150.67	Joback Method
cpg	1379.34	J/mol×K	1188.20	Joback Method
cpg	1389.27	J/mol×K	1225.74	Joback Method
dvisc	0.0003310	Pa×s	547.31	Joback Method

dvisc	0.0001475	Pa×s	622.84	Joback Method
dvisc	0.0000783	Pa×s	698.38	Joback Method
dvisc	0.0000470	Pa×s	773.91	Joback Method
dvisc	0.0000309	Pa×s	849.45	Joback Method
dvisc	0.0000218	Pa×s	924.99	Joback Method
dvisc	0.0000162	Pa×s	1000.52	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=U383005&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