Terephthalic acid, dodecyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C26H42O4/c1-5-7-8-9-10-11-12-13-14-15-20-29-25(27)22-16-18-23(19-17-22)26(28)30-24(6-2)21(3)4/h16-19,21,24H,5-15,20H2,1-4H3

InchiKey: DLLJDYCLMZWQAO-UHFFFAOYSA-N

Formula: C26H42O4

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

Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-201.90	kJ/mol	Joback Method
hf	-855.07	kJ/mol	Joback Method
hfus	55.28	kJ/mol	Joback Method
hvap	93.94	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.356		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	923.86	kPa	Joback Method
rinpol	2957.00		NIST Webbook
rinpol	2957.00		NIST Webbook
tb	977.64	K	Joback Method
tc	1196.94	K	Joback Method
tf	536.04	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.40	J/mol×K	977.64	Joback Method
cpg	1316.39	J/mol×K	1160.39	Joback Method
cpg	1304.91	J/mol×K	1123.84	Joback Method
cpg	1292.02	J/mol×K	1087.29	Joback Method
cpg	1277.68	J/mol×K	1050.74	Joback Method
cpg	1261.82	J/mol×K	1014.19	Joback Method
cpg	1326.50	J/mol×K	1196.94	Joback Method
dvisc	0.0000189	Pa×s	977.64	Joback Method

dvisc	0.0000254	Pa×s	904.04	Joback Method
dvisc	0.0000360	Pa×s	830.44	Joback Method
dvisc	0.0000545	Pa×s	756.84	Joback Method
dvisc	0.0000904	Pa×s	683.24	Joback Method
dvisc	0.0001694	Pa×s	609.64	Joback Method
dvisc	0.0003771	Pa×s	536.04	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=U356203&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