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

Inchi: InChI=1S/C25H40O4/c1-5-6-7-8-9-10-11-12-13-14-19-28-24(26)22-15-17-23(18-16-22)25(27)29-20-21(2)3/h15-18,21H,5-14,19-20H2,1-4H3

InchiKey: OPFZWEGVGLPWJE-UHFFFAOYSA-N

Formula: C25H40O4

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

Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-210.32	kJ/mol	Joback Method
hf	-834.43	kJ/mol	Joback Method
hfus	52.69	kJ/mol	Joback Method
hvap	91.72	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	6.966		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	980.23	kPa	Joback Method
rinpol	2889.00		NIST Webbook
tb	954.76	K	Joback Method
tc	1169.19	K	Joback Method
tf	524.77	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.11	J/mol×K	954.76	Joback Method
cpg	1199.33	J/mol×K	990.50	Joback Method
cpg	1215.06	J/mol×K	1026.24	Joback Method
cpg	1229.37	J/mol×K	1061.98	Joback Method
cpg	1242.28	J/mol×K	1097.71	Joback Method
cpg	1253.86	J/mol×K	1133.45	Joback Method
cpg	1264.13	J/mol×K	1169.19	Joback Method
dvisc	0.0004286	Pa×s	524.77	Joback Method
dvisc	0.0001941	Pa×s	596.43	Joback Method

dvisc	0.0001042	Pa×s	668.10	Joback Method
dvisc	0.0000631	Pa×s	739.76	Joback Method
dvisc	0.0000418	Pa×s	811.43	Joback Method
dvisc	0.0000295	Pa×s	883.09	Joback Method
dvisc	0.0000220	Pa×s	954.76	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=U356280&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