Terephthalic acid, dodecyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C28H46O4/c1-6-7-8-9-10-11-12-13-14-15-20-31-26(29)24-16-18-25(19-17-24)28(30)32-21-23(5)22-27(2,3)4/h16-19,23H,6-15,20-22H2,1-5H3

InchiKey: OAXUPECMUBLCEG-UHFFFAOYSA-N

Formula: C28H46O4

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

Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-179.78	kJ/mol	Joback Method
hf	-899.82	kJ/mol	Joback Method
hfus	56.57	kJ/mol	Joback Method
hvap	97.49	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	7.993		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	830.02	kPa	Joback Method
rinpol	3277.00		NIST Webbook
rinpol	3277.00		NIST Webbook
tb	1020.61	K	Joback Method
tc	1250.70	K	Joback Method
tf	576.00	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.73	J/mol×K	1020.61	Joback Method
cpg	1445.19	J/mol×K	1212.35	Joback Method
cpg	1432.88	J/mol×K	1174.00	Joback Method
cpg	1419.26	J/mol×K	1135.65	Joback Method
cpg	1404.26	J/mol×K	1097.31	Joback Method
cpg	1387.78	J/mol×K	1058.96	Joback Method
cpg	1456.30	J/mol×K	1250.70	Joback Method
dvisc	0.0000114	Pa×s	1020.61	Joback Method

dvisc	0.0000155	Pa×s	946.51	Joback Method
dvisc	0.0000220	Pa×s	872.41	Joback Method
dvisc	0.0000335	Pa×s	798.31	Joback Method
dvisc	0.0000556	Pa×s	724.20	Joback Method
dvisc	0.0001033	Pa×s	650.10	Joback Method
dvisc	0.0002256	Pa×s	576.00	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=U416018&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