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

Inchi: InChI=1S/C27H44O4/c1-6-7-8-9-10-11-12-13-14-19-30-25(28)23-15-17-24(18-16-23)26(

InchiKey: FVGOFTJBROPKKV-UHFFFAOYSA-N

Formula: C27H44O4

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

Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-188.20	kJ/mol	Joback Method
hf	-879.18	kJ/mol	Joback Method
hfus	53.98	kJ/mol	Joback Method
hvap	95.26	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	7.603		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
rinpol	3177.00		NIST Webbook
rinpol	3177.00		NIST Webbook
tb	997.73	K	Joback Method
tc	1221.62	K	Joback Method
tf	564.73	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.64	J/mol×K	997.73	Joback Method
cpg	1381.24	J/mol×K	1184.30	Joback Method
cpg	1368.98	J/mol×K	1146.99	Joback Method
cpg	1355.47	J/mol×K	1109.67	Joback Method
cpg	1340.63	J/mol×K	1072.36	Joback Method
cpg	1324.38	J/mol×K	1035.04	Joback Method
cpg	1392.33	J/mol×K	1221.62	Joback Method
dvisc	0.0000134	Pa×s	997.73	Joback Method

dvisc	0.0000181	Pa×s	925.56	Joback Method
dvisc	0.0000258	Pa×s	853.40	Joback Method
dvisc	0.0000391	Pa×s	781.23	Joback Method
dvisc	0.0000646	Pa×s	709.06	Joback Method
dvisc	0.0001195	Pa×s	636.90	Joback Method
dvisc	0.0002587	Pa×s	564.73	Joback Method

Sources

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=U416017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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