Terephthalic acid, 2-heptyl pentadecyl ester

Inchi: InChI=1S/C30H50O4/c1-4-6-8-9-10-11-12-13-14-15-16-17-19-25-33-29(31)27-21-23-28(
InchiKey: XIGWJGPSMVGWAV-UHFFFAOYSA-N
Formula: C30H50O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(C)CCCCC)cc1
Mol. weight [g/mol]: 474.72

Physical Properties

Property code	Value	Unit	Source
gf	-165.78	kJ/mol	Joback Method
hf	-932.35	kJ/mol	Joback Method
hfus	69.16	kJ/mol	Joback Method
hvap	103.24	kJ/mol	Joback Method
log10ws	-10.44		Crippen Method
logp	9.060		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	737.62	kPa	Joback Method
rinpol	3403.00		NIST Webbook
rinpol	3403.00		NIST Webbook
tb	1069.60	K	Joback Method
tc	1321.85	K	Joback Method
tf	596.12	K	Joback Method
vc	1.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.00	J/mol×K	1069.60	Joback Method
cpg	1515.79	J/mol×K	1111.64	Joback Method
cpg	1532.50	J/mol×K	1153.68	Joback Method
cpg	1547.22	J/mol×K	1195.73	Joback Method
cpg	1560.06	J/mol×K	1237.77	Joback Method
cpg	1571.11	J/mol×K	1279.81	Joback Method
cpg	1580.48	J/mol×K	1321.85	Joback Method
dvisc	0.0001997	Pa×s	596.12	Joback Method

dvisc	0.0000931	Pa×s	675.03	Joback Method
dvisc	0.0000509	Pa×s	753.95	Joback Method
dvisc	0.0000312	Pa×s	832.86	Joback Method
dvisc	0.0000208	Pa×s	911.77	Joback Method
dvisc	0.0000148	Pa×s	990.69	Joback Method
dvisc	0.0000111	Pa×s	1069.60	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=U356299&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