Phthalic acid, 2-methylbenzyl tridecyl ester

Inchi: InChI=1S/C29H40O4/c1-3-4-5-6-7-8-9-10-11-12-17-22-32-28(30)26-20-15-16-21-27(26)2
InchiKey: MSEWIKZOPVOCSX-UHFFFAOYSA-N
Formula: C29H40O4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C
Mol. weight [g/mol]: 452.63

Physical Properties

Property code	Value	Unit	Source
gf	-68.98	kJ/mol	Joback Method
hf	-681.37	kJ/mol	Joback Method
hfus	63.74	kJ/mol	Joback Method
hvap	104.34	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	7.820		Crippen Method
mcvol	386.830	ml/mol	McGowan Method
pc	930.64	kPa	Joback Method
rinpol	3265.00		NIST Webbook
rinpol	3265.00		NIST Webbook
tb	1078.82	K	Joback Method
tc	1321.69	K	Joback Method
tf	638.79	K	Joback Method
vc	1.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1321.30	J/mol×K	1078.82	Joback Method
cpg	1336.02	J/mol×K	1119.30	Joback Method
cpg	1349.02	J/mol×K	1159.78	Joback Method
cpg	1360.37	J/mol×K	1200.26	Joback Method
cpg	1370.17	J/mol×K	1240.74	Joback Method
cpg	1378.49	J/mol×K	1281.22	Joback Method
cpg	1385.41	J/mol×K	1321.69	Joback Method
dvisc	0.0001676	Pa×s	638.79	Joback Method

dvisc	0.0000917	Pa×s	712.13	Joback Method
dvisc	0.0000561	Pa×s	785.47	Joback Method
dvisc	0.0000374	Pa×s	858.81	Joback Method
dvisc	0.0000265	Pa×s	932.14	Joback Method
dvisc	0.0000198	Pa×s	1005.48	Joback Method
dvisc	0.0000154	Pa×s	1078.82	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=U382859&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