Phthalic acid, 2-methoxybenzyl tridecyl ester

Inchi: InChI=1S/C29H40O5/c1-3-4-5-6-7-8-9-10-11-12-17-22-33-28(30)25-19-14-15-20-26(25)2
InchiKey: HOLGMNXKQOSTDA-UHFFFAOYSA-N
Formula: C29H40O5
SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1OC
Mol. weight [g/mol]: 468.62

Physical Properties

Property code	Value	Unit	Source
gf	-173.98	kJ/mol	Joback Method
hf	-813.59	kJ/mol	Joback Method
hfus	64.93	kJ/mol	Joback Method
hvap	106.75	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	7.520		Crippen Method
mcvol	392.700	ml/mol	McGowan Method
pc	921.06	kPa	Joback Method
rinpol	3872.00		NIST Webbook
rinpol	3872.00		NIST Webbook
tb	1101.24	K	Joback Method
tc	1350.95	K	Joback Method
tf	661.02	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.00	J/mol×K	1101.24	Joback Method
cpg	1393.48	J/mol×K	1309.33	Joback Method
cpg	1387.99	J/mol×K	1267.72	Joback Method
cpg	1380.67	J/mol×K	1226.10	Joback Method
cpg	1371.44	J/mol×K	1184.48	Joback Method
cpg	1360.24	J/mol×K	1142.86	Joback Method
cpg	1397.19	J/mol×K	1350.95	Joback Method
dvisc	0.0000113	Pa×s	1101.24	Joback Method

dvisc	0.0000145	Pa×s	1027.87	Joback Method
dvisc	0.0000193	Pa×s	954.50	Joback Method
dvisc	0.0000270	Pa×s	881.13	Joback Method
dvisc	0.0000403	Pa×s	807.76	Joback Method
dvisc	0.0000650	Pa×s	734.39	Joback Method
dvisc	0.0001165	Pa×s	661.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382502&Units=SI
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

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