Phthalic acid, 4-chloro-2-methoxybenzyl undecyl ester

Inchi: InChI=1S/C27H35ClO5/c1-3-4-5-6-7-8-9-10-13-18-32-26(29)23-14-11-12-15-24(23)27(30

InchiKey: UEYPMKNSBXRJBJ-UHFFFAOYSA-N

Formula: C27H35ClO5

SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 475.02

Physical Properties

Property code	Value	Unit	Source
gf	-212.38	kJ/mol	Joback Method
hf	-799.52	kJ/mol	Joback Method
hfus	63.56	kJ/mol	Joback Method
hvap	107.34	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	7.393		Crippen Method
mcvol	376.760	ml/mol	McGowan Method
pc	1004.62	kPa	Joback Method
rinpol	3370.00		NIST Webbook
rinpol	3370.00		NIST Webbook
tb	1097.89	K	Joback Method
tc	1344.74	K	Joback Method
tf	680.92	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.22	J/mol×K	1097.89	Joback Method
cpg	1281.66	J/mol×K	1303.60	Joback Method
cpg	1277.64	J/mol×K	1262.46	Joback Method
cpg	1271.84	J/mol×K	1221.32	Joback Method
cpg	1264.20	J/mol×K	1180.17	Joback Method
cpg	1254.67	J/mol×K	1139.03	Joback Method
cpg	1283.93	J/mol×K	1344.74	Joback Method
dvisc	0.0000132	Pa×s	1097.89	Joback Method

dvisc	0.0000167	Pa×s	1028.39	Joback Method
dvisc	0.0000218	Pa×s	958.90	Joback Method
dvisc	0.0000297	Pa×s	889.41	Joback Method
dvisc	0.0000427	Pa×s	819.91	Joback Method
dvisc	0.0000655	Pa×s	750.42	Joback Method
dvisc	0.0001098	Pa×s	680.92	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=U382845&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