Phthalic acid, 2,5-dichlorophenyl tridecyl ester

Inchi: InChI=1S/C27H34Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-14-19-32-26(30)22-15-12-13-16-23(22
InchiKey: JSZSFCYVCPSVPH-UHFFFAOYSA-N
Formula: C27H34Cl2O4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 493.46

Physical Properties

Property code	Value	Unit	Source
gf	-119.31	kJ/mol	Joback Method
hf	-683.04	kJ/mol	Joback Method
hfus	66.57	kJ/mol	Joback Method
hvap	109.32	kJ/mol	Joback Method
log10ws	-10.19		Crippen Method
logp	8.680		Crippen Method
mcvol	383.130	ml/mol	McGowan Method
pc	992.00	kPa	Joback Method
rinpol	3494.00		NIST Webbook
tb	1112.90	K	Joback Method
tc	1363.04	K	Joback Method
tf	688.61	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.09	J/mol×K	1112.90	Joback Method
cpg	1249.72	J/mol×K	1154.59	Joback Method
cpg	1259.70	J/mol×K	1196.28	Joback Method
cpg	1268.10	J/mol×K	1237.97	Joback Method
cpg	1275.00	J/mol×K	1279.66	Joback Method
cpg	1280.47	J/mol×K	1321.35	Joback Method
cpg	1284.61	J/mol×K	1363.04	Joback Method
dvisc	0.0001262	Pa×s	688.61	Joback Method
dvisc	0.0000750	Pa×s	759.33	Joback Method

dvisc	0.0000487	Pa×s	830.04	Joback Method
dvisc	0.0000339	Pa×s	900.76	Joback Method
dvisc	0.0000248	Pa×s	971.47	Joback Method
dvisc	0.0000190	Pa×s	1042.18	Joback Method
dvisc	0.0000150	Pa×s	1112.90	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=U356663&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