Phthalic acid, 2-(2-fluorophenyl)ethyl undecyl ester

Inchi: InChI=1S/C27H35FO4/c1-2-3-4-5-6-7-8-9-14-20-31-26(29)23-16-11-12-17-24(23)27(30)3

InchiKey: BWKJITOUMQZQAM-UHFFFAOYSA-N

Formula: C27H35FO4

SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccccc1F

Mol. weight [g/mol]: 442.56

Physical Properties

Property code	Value	Unit	Source
gf	-280.63	kJ/mol	Joback Method
hf	-836.20	kJ/mol	Joback Method
hfus	61.64	kJ/mol	Joback Method
hvap	99.07	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	6.913		Crippen Method
mcvol	360.420	ml/mol	McGowan Method
pc	1020.08	kPa	Joback Method
rinpol	3169.00		NIST Webbook
rinpol	3169.00		NIST Webbook
tb	1032.33	K	Joback Method
tc	1263.87	K	Joback Method
tf	616.84	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1204.53	J/mol×K	1032.33	Joback Method
cpg	1218.88	J/mol×K	1070.92	Joback Method
cpg	1231.68	J/mol×K	1109.51	Joback Method
cpg	1242.99	J/mol×K	1148.10	Joback Method
cpg	1252.87	J/mol×K	1186.69	Joback Method
cpg	1261.39	J/mol×K	1225.28	Joback Method
cpg	1268.61	J/mol×K	1263.87	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=U378057&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
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