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

Inchi: InChI=1S/C31H43FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-24-35-30(33)27-20-15-16-21-2

InchiKey: XVWFZFNKGZFTLU-UHFFFAOYSA-N

Formula: C31H43FO4

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

Mol. weight [g/mol]: 498.67

Physical Properties

Property code	Value	Unit	Source
gf	-246.95	kJ/mol	Joback Method
hf	-918.76	kJ/mol	Joback Method
hfus	72.00	kJ/mol	Joback Method
hvap	107.97	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	8.473		Crippen Method
mcvol	416.780	ml/mol	McGowan Method
pc	809.37	kPa	Joback Method
rinpol	3577.00		NIST Webbook
rinpol	3577.00		NIST Webbook
tb	1123.85	K	Joback Method
tc	1386.10	K	Joback Method
tf	661.92	K	Joback Method
vc	1.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1452.21	J/mol×K	1123.85	Joback Method
cpg	1467.31	J/mol×K	1167.56	Joback Method
cpg	1480.43	J/mol×K	1211.27	Joback Method
cpg	1491.69	J/mol×K	1254.98	Joback Method
cpg	1501.20	J/mol×K	1298.68	Joback Method
cpg	1509.09	J/mol×K	1342.39	Joback Method
cpg	1515.47	J/mol×K	1386.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378061&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
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

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