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

Inchi: InChI=1S/C33H47FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-26-37-32(35)29-22-17-1

InchiKey: XHAZLPMDZAMXFL-UHFFFAOYSA-N

Formula: C33H47FO4

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

Mol. weight [g/mol]: 526.72

Physical Properties

Property code	Value	Unit	Source
gf	-230.11	kJ/mol	Joback Method
hf	-960.04	kJ/mol	Joback Method
hfus	77.18	kJ/mol	Joback Method
hvap	112.42	kJ/mol	Joback Method
log10ws	-11.02		Crippen Method
logp	9.253		Crippen Method
mcvol	444.960	ml/mol	McGowan Method
pc	727.70	kPa	Joback Method
rinpol	3776.00		NIST Webbook
tb	1169.61	K	Joback Method
tc	1455.62	K	Joback Method
tf	684.46	K	Joback Method
vc	1.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1577.62	J/mol×K	1169.61	Joback Method
cpg	1593.26	J/mol×K	1217.28	Joback Method
cpg	1606.61	J/mol×K	1264.95	Joback Method
cpg	1617.83	J/mol×K	1312.62	Joback Method
cpg	1627.10	J/mol×K	1360.28	Joback Method
cpg	1634.58	J/mol×K	1407.95	Joback Method
cpg	1640.44	J/mol×K	1455.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378063&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