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

Inchi: InChI=1S/C23H27FO4/c1-2-3-4-5-10-16-27-22(25)19-12-7-8-13-20(19)23(26)28-17-15-1

InchiKey: VNWFLCBEYWGMCC-UHFFFAOYSA-N

Formula: C23H27FO4

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

Mol. weight [g/mol]: 386.46

Physical Properties

Property code	Value	Unit	Source
gf	-314.31	kJ/mol	Joback Method
hf	-753.64	kJ/mol	Joback Method
hfus	51.28	kJ/mol	Joback Method
hvap	90.16	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.352		Crippen Method
mcvol	304.060	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	2764.00		NIST Webbook
rinpol	2764.00		NIST Webbook
tb	940.81	K	Joback Method
tc	1159.53	K	Joback Method
tf	571.76	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.99	J/mol×K	940.81	Joback Method
cpg	976.89	J/mol×K	977.26	Joback Method
cpg	989.48	J/mol×K	1013.72	Joback Method
cpg	1000.79	J/mol×K	1050.17	Joback Method
cpg	1010.85	J/mol×K	1086.62	Joback Method
cpg	1019.72	J/mol×K	1123.07	Joback Method
cpg	1027.43	J/mol×K	1159.53	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378054&Units=SI

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