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

Inchi: InChI=1S/C21H23FO4/c1-2-3-8-14-25-20(23)17-10-5-6-11-18(17)21(24)26-15-13-16-9-4

InchiKey: AGRRSFMQWGHYHP-UHFFFAOYSA-N

Formula: C21H23FO4

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

Mol. weight [g/mol]: 358.40

Physical Properties

Property code	Value	Unit	Source
gf	-331.15	kJ/mol	Joback Method
hf	-712.36	kJ/mol	Joback Method
hfus	46.10	kJ/mol	Joback Method
hvap	85.71	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.572		Crippen Method
mcvol	275.880	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	2565.00		NIST Webbook
tb	895.05	K	Joback Method
tc	1112.73	K	Joback Method
tf	549.22	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.44	J/mol×K	895.05	Joback Method
cpg	859.16	J/mol×K	931.33	Joback Method
cpg	871.62	J/mol×K	967.61	Joback Method
cpg	882.86	J/mol×K	1003.89	Joback Method
cpg	892.93	J/mol×K	1040.17	Joback Method
cpg	901.84	J/mol×K	1076.45	Joback Method
cpg	909.65	J/mol×K	1112.73	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=U378052&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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