Phthalic acid, 2,5-difluorobenzyl pentadecyl ester

Inchi: InChI=1S/C30H40F2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-21-35-29(33)26-17-14-15-18

InchiKey: VXUALWDTENYEIQ-UHFFFAOYSA-N

Formula: C30H40F2O4

SMILES: CCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1F

Mol. weight [g/mol]: 502.63

Physical Properties

Property code	Value	Unit	Source
gf	-459.81	kJ/mol	Joback Method
hf	-1105.70	kJ/mol	Joback Method
hfus	72.11	kJ/mol	Joback Method
hvap	105.59	kJ/mol	Joback Method
log10ws	-10.59		Crippen Method
logp	8.570		Crippen Method
mcvol	404.460	ml/mol	McGowan Method
pc	826.21	kPa	Joback Method
rinpol	3351.00		NIST Webbook
rinpol	3351.00		NIST Webbook
tb	1105.22	K	Joback Method
tc	1362.68	K	Joback Method
tf	663.76	K	Joback Method
vc	1.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.91	J/mol×K	1105.22	Joback Method
cpg	1409.55	J/mol×K	1148.13	Joback Method
cpg	1422.23	J/mol×K	1191.04	Joback Method
cpg	1433.03	J/mol×K	1233.95	Joback Method
cpg	1442.06	J/mol×K	1276.86	Joback Method
cpg	1449.41	J/mol×K	1319.77	Joback Method
cpg	1455.18	J/mol×K	1362.68	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=U377812&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