Phthalic acid, 2,5-difluorobenzyl dodecyl ester

Inchi: InChI=1S/C27H34F2O4/c1-2-3-4-5-6-7-8-9-10-13-18-32-26(30)23-14-11-12-15-24(23)27
InchiKey: ANJMJXIALAIWJA-UHFFFAOYSA-N
Formula: C27H34F2O4
SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 460.55

Physical Properties

Property code	Value	Unit	Source
gf	-485.07	kJ/mol	Joback Method
hf	-1043.78	kJ/mol	Joback Method
hfus	64.34	kJ/mol	Joback Method
hvap	98.91	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	7.400		Crippen Method
mcvol	362.190	ml/mol	McGowan Method
pc	982.08	kPa	Joback Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tb	1036.58	K	Joback Method
tc	1269.63	K	Joback Method
tf	629.95	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1210.05	J/mol×K	1036.58	Joback Method
cpg	1224.11	J/mol×K	1075.42	Joback Method
cpg	1236.57	J/mol×K	1114.26	Joback Method
cpg	1247.48	J/mol×K	1153.11	Joback Method
cpg	1256.90	J/mol×K	1191.95	Joback Method
cpg	1264.91	J/mol×K	1230.79	Joback Method
cpg	1271.55	J/mol×K	1269.63	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=U377809&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