Phthalic acid, 2,5-difluorobenzyl tridecyl ester

Inchi: InChI=1S/C28H36F2O4/c1-2-3-4-5-6-7-8-9-10-11-14-19-33-27(31)24-15-12-13-16-25(24
InchiKey: RXGJLVUCRDLHOF-UHFFFAOYSA-N
Formula: C28H36F2O4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 474.58

Physical Properties

Property code	Value	Unit	Source
gf	-476.65	kJ/mol	Joback Method
hf	-1064.42	kJ/mol	Joback Method
hfus	66.93	kJ/mol	Joback Method
hvap	101.14	kJ/mol	Joback Method
log10ws	-9.75		Crippen Method
logp	7.790		Crippen Method
mcvol	376.280	ml/mol	McGowan Method
pc	925.55	kPa	Joback Method
rinpol	3144.00		NIST Webbook
rinpol	3144.00		NIST Webbook
tb	1059.46	K	Joback Method
tc	1299.37	K	Joback Method
tf	641.22	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1271.36	J/mol×K	1059.46	Joback Method
cpg	1285.60	J/mol×K	1099.45	Joback Method
cpg	1298.12	J/mol×K	1139.43	Joback Method
cpg	1309.01	J/mol×K	1179.42	Joback Method
cpg	1318.33	J/mol×K	1219.40	Joback Method
cpg	1326.14	J/mol×K	1259.39	Joback Method
cpg	1332.53	J/mol×K	1299.37	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=U377810&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