Phthalic acid, 2,5-difluorobenzyl hexadecyl ester

Inchi: InChI=1S/C31H42F2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-22-36-30(34)27-18-15-16

InchiKey: NIMSNKQNNJDZNH-UHFFFAOYSA-N

Formula: C31H42F2O4

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

Mol. weight [g/mol]: 516.66

Physical Properties

Property code	Value	Unit	Source
gf	-451.39	kJ/mol	Joback Method
hf	-1126.34	kJ/mol	Joback Method
hfus	74.70	kJ/mol	Joback Method
hvap	107.82	kJ/mol	Joback Method
log10ws	-11.01		Crippen Method
logp	8.960		Crippen Method
mcvol	418.550	ml/mol	McGowan Method
pc	782.43	kPa	Joback Method
rinpol	3454.00		NIST Webbook
tb	1128.10	K	Joback Method
tc	1396.44	K	Joback Method
tf	675.03	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1457.08	J/mol×K	1128.10	Joback Method
cpg	1471.96	J/mol×K	1172.82	Joback Method
cpg	1484.71	J/mol×K	1217.55	Joback Method
cpg	1495.44	J/mol×K	1262.27	Joback Method
cpg	1504.28	J/mol×K	1307.00	Joback Method
cpg	1511.35	J/mol×K	1351.72	Joback Method
cpg	1516.75	J/mol×K	1396.44	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=U377813&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