Phthalic acid, 2-bromo-5-fluorobenzyl tridecyl ester

Inchi: InChI=1S/C28H36BrFO4/c1-2-3-4-5-6-7-8-9-10-11-14-19-33-27(31)24-15-12-13-16-25(2

InchiKey: OIQITNGGQNQCAE-UHFFFAOYSA-N

Formula: C28H36BrFO4

SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1Br

Mol. weight [g/mol]: 535.49

Physical Properties

Property code	Value	Unit	Source
gf	-267.52	kJ/mol	Joback Method
hf	-841.98	kJ/mol	Joback Method
hfus	69.13	kJ/mol	Joback Method
hvap	108.39	kJ/mol	Joback Method
log10ws	-10.58		Crippen Method
logp	8.413		Crippen Method
mcvol	392.010	ml/mol	McGowan Method
pc	993.25	kPa	Joback Method
rinpol	3896.00		NIST Webbook
tb	1126.35	K	Joback Method
tc	1381.70	K	Joback Method
tf	700.43	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1296.99	J/mol×K	1126.35	Joback Method
cpg	1309.63	J/mol×K	1168.91	Joback Method
cpg	1320.63	J/mol×K	1211.47	Joback Method
cpg	1330.10	J/mol×K	1254.03	Joback Method
cpg	1338.12	J/mol×K	1296.58	Joback Method
cpg	1344.80	J/mol×K	1339.14	Joback Method
cpg	1350.24	J/mol×K	1381.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382516&Units=SI
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

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