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

Inchi: InChI=1S/C25H30BrFO4/c1-2-3-4-5-6-7-8-11-16-30-24(28)21-12-9-10-13-22(21)25(29)3

InchiKey: JDDBMMULKIAOAL-UHFFFAOYSA-N

Formula: C25H30BrFO4

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

Mol. weight [g/mol]: 493.41

Physical Properties

Property code	Value	Unit	Source
gf	-292.78	kJ/mol	Joback Method
hf	-780.06	kJ/mol	Joback Method
hfus	61.36	kJ/mol	Joback Method
hvap	101.71	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	7.243		Crippen Method
mcvol	349.740	ml/mol	McGowan Method
pc	1201.46	kPa	Joback Method
rinpol	3596.00		NIST Webbook
rinpol	3596.00		NIST Webbook
tb	1057.71	K	Joback Method
tc	1295.37	K	Joback Method
tf	666.62	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1114.53	J/mol×K	1057.71	Joback Method
cpg	1126.71	J/mol×K	1097.32	Joback Method
cpg	1137.48	J/mol×K	1136.93	Joback Method
cpg	1146.90	J/mol×K	1176.54	Joback Method
cpg	1155.03	J/mol×K	1216.15	Joback Method
cpg	1161.95	J/mol×K	1255.76	Joback Method
cpg	1167.71	J/mol×K	1295.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382513&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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