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

Inchi: InChI=1S/C22H24BrFO4/c1-2-3-4-5-8-13-27-21(25)18-9-6-7-10-19(18)22(26)28-15-16-14

InchiKey: VKXHBLKHEMXOLV-UHFFFAOYSA-N

Formula: C22H24BrFO4

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

Mol. weight [g/mol]: 451.33

Physical Properties

Property code	Value	Unit	Source
gf	-318.04	kJ/mol	Joback Method
hf	-718.14	kJ/mol	Joback Method
hfus	53.59	kJ/mol	Joback Method
hvap	95.03	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	6.072		Crippen Method
mcvol	307.470	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpol	3294.00		NIST Webbook
rinpol	3294.00		NIST Webbook
tb	989.07	K	Joback Method
tc	1218.90	K	Joback Method
tf	632.81	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.82	J/mol×K	989.07	Joback Method
cpg	947.67	J/mol×K	1027.37	Joback Method
cpg	958.24	J/mol×K	1065.68	Joback Method
cpg	967.58	J/mol×K	1103.98	Joback Method
cpg	975.75	J/mol×K	1142.29	Joback Method
cpg	982.77	J/mol×K	1180.59	Joback Method
cpg	988.71	J/mol×K	1218.90	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=U382510&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