Succinic acid, 2-bromo-4-fluorophenyl 2-biphenyl ester

Inchi: InChI=1S/C22H16BrFO4/c23-18-14-16(24)10-11-20(18)28-22(26)13-12-21(25)27-19-9-5

InchiKey: YFXDANIOBZWOBA-UHFFFAOYSA-N

Formula: C22H16BrFO4

SMILES: O=C(CCC(=O)Oc1ccccc1-c1ccccc1)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 443.26

Physical Properties

Property code	Value	Unit	Source
gf	-205.63	kJ/mol	Joback Method
hf	-481.61	kJ/mol	Joback Method
hfus	47.63	kJ/mol	Joback Method
hvap	97.31	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	5.546		Crippen Method
mcvol	283.710	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	3038.00		NIST Webbook
rinpol	3038.00		NIST Webbook
tb	1015.75	K	Joback Method
tc	1268.41	K	Joback Method
tf	659.23	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.68	J/mol×K	1015.75	Joback Method
cpg	834.07	J/mol×K	1057.86	Joback Method
cpg	842.14	J/mol×K	1099.97	Joback Method
cpg	848.96	J/mol×K	1142.08	Joback Method
cpg	854.61	J/mol×K	1184.19	Joback Method
cpg	859.16	J/mol×K	1226.30	Joback Method
cpg	862.69	J/mol×K	1268.41	Joback Method

Sources

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=U358019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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