Sebacic acid, 2-bromo-4-fluorophenyl isohexyl ester

Inchi: InChI=1S/C22H32BrFO4/c1-17(2)10-9-15-27-21(25)11-7-5-3-4-6-8-12-22(26)28-20-14-13

InchiKey: JQPJFUKMAXOPBU-UHFFFAOYSA-N

Formula: C22H32BrFO4

SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 459.39

Physical Properties

Property code	Value	Unit	Source
gf	-423.26	kJ/mol	Joback Method
hf	-948.48	kJ/mol	Joback Method
hfus	56.41	kJ/mol	Joback Method
hvap	91.71	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.594		Crippen Method
mcvol	331.230	ml/mol	McGowan Method
pc	1184.97	kPa	Joback Method
rinpol	2918.00		NIST Webbook
rinpol	2918.00		NIST Webbook
tb	956.97	K	Joback Method
tc	1172.77	K	Joback Method
tf	578.87	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.20	J/mol×K	956.97	Joback Method
cpg	1058.74	J/mol×K	992.94	Joback Method
cpg	1072.00	J/mol×K	1028.90	Joback Method
cpg	1084.04	J/mol×K	1064.87	Joback Method
cpg	1094.88	J/mol×K	1100.83	Joback Method
cpg	1104.57	J/mol×K	1136.80	Joback Method
cpg	1113.14	J/mol×K	1172.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354554&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