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

Inchi: InChI=1S/C23H34BrFO4/c1-2-3-4-9-12-17-28-22(26)13-10-7-5-6-8-11-14-23(27)29-21-1

InchiKey: TVURTGRHOFDBMJ-UHFFFAOYSA-N

Formula: C23H34BrFO4

SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 473.42

Physical Properties

Property code	Value	Unit	Source
gf	-412.40	kJ/mol	Joback Method
hf	-963.84	kJ/mol	Joback Method
hfus	62.53	kJ/mol	Joback Method
hvap	94.32	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	7.128		Crippen Method
mcvol	345.320	ml/mol	McGowan Method
pc	1104.47	kPa	Joback Method
rinpol	3075.00		NIST Webbook
rinpol	3075.00		NIST Webbook
tb	980.29	K	Joback Method
tc	1200.16	K	Joback Method
tf	605.14	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.35	J/mol×K	980.29	Joback Method
cpg	1119.18	J/mol×K	1016.93	Joback Method
cpg	1132.69	J/mol×K	1053.58	Joback Method
cpg	1144.91	J/mol×K	1090.22	Joback Method
cpg	1155.89	J/mol×K	1126.87	Joback Method
cpg	1165.67	J/mol×K	1163.51	Joback Method
cpg	1174.31	J/mol×K	1200.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354556&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