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

Inchi: InChI=1S/C27H42BrFO4/c1-2-3-4-5-6-7-10-13-16-21-32-26(30)17-14-11-8-9-12-15-18-2

InchiKey: GWRVCOQOLBRVBQ-UHFFFAOYSA-N

Formula: C27H42BrFO4

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

Mol. weight [g/mol]: 529.52

Physical Properties

Property code	Value	Unit	Source
gf	-378.72	kJ/mol	Joback Method
hf	-1046.40	kJ/mol	Joback Method
hfus	72.89	kJ/mol	Joback Method
hvap	103.23	kJ/mol	Joback Method
log10ws	-10.10		Crippen Method
logp	8.688		Crippen Method
mcvol	401.680	ml/mol	McGowan Method
pc	868.62	kPa	Joback Method
rinpol	3500.00		NIST Webbook
rinpol	3500.00		NIST Webbook
tb	1071.81	K	Joback Method
tc	1320.88	K	Joback Method
tf	650.22	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1351.21	J/mol×K	1071.81	Joback Method
cpg	1367.37	J/mol×K	1113.32	Joback Method
cpg	1381.77	J/mol×K	1154.83	Joback Method
cpg	1394.50	J/mol×K	1196.35	Joback Method
cpg	1405.65	J/mol×K	1237.86	Joback Method
cpg	1415.29	J/mol×K	1279.37	Joback Method
cpg	1423.51	J/mol×K	1320.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354560&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