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

Inchi: InChI=1S/C28H44BrFO4/c1-2-3-4-5-6-7-8-11-14-17-22-33-27(31)18-15-12-9-10-13-16-19

InchiKey: YOAILTRUFCRJBY-UHFFFAOYSA-N

Formula: C28H44BrFO4

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

Mol. weight [g/mol]: 543.55

Physical Properties

Property code	Value	Unit	Source
gf	-370.30	kJ/mol	Joback Method
hf	-1067.04	kJ/mol	Joback Method
hfus	75.48	kJ/mol	Joback Method
hvap	105.45	kJ/mol	Joback Method
log10ws	-10.51		Crippen Method
logp	9.079		Crippen Method
mcvol	415.770	ml/mol	McGowan Method
pc	821.48	kPa	Joback Method
rinpol	3618.00		NIST Webbook
rinpol	3618.00		NIST Webbook
tb	1094.69	K	Joback Method
tc	1354.30	K	Joback Method
tf	661.49	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1413.85	J/mol×K	1094.69	Joback Method
cpg	1430.41	J/mol×K	1137.96	Joback Method
cpg	1445.07	J/mol×K	1181.23	Joback Method
cpg	1457.93	J/mol×K	1224.50	Joback Method
cpg	1469.08	J/mol×K	1267.76	Joback Method
cpg	1478.64	J/mol×K	1311.03	Joback Method
cpg	1486.69	J/mol×K	1354.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354561&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