Sebacic acid, 2-bromo-5-fluorobenzyl pentyl ester

Inchi: InChI=1S/C22H32BrFO4/c1-2-3-10-15-27-21(25)11-8-6-4-5-7-9-12-22(26)28-17-18-16-19

InchiKey: JQFCHXLQQKLBEO-UHFFFAOYSA-N

Formula: C22H32BrFO4

SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCc1cc(F)ccc1Br

Mol. weight [g/mol]: 459.39

Physical Properties

Property code	Value	Unit	Source
gf	-420.82	kJ/mol	Joback Method
hf	-943.20	kJ/mol	Joback Method
hfus	59.94	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	6.486		Crippen Method
mcvol	331.230	ml/mol	McGowan Method
pc	1178.47	kPa	Joback Method
rinpol	2914.00		NIST Webbook
rinpol	2914.00		NIST Webbook
tb	957.41	K	Joback Method
tc	1172.78	K	Joback Method
tf	593.87	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.77	J/mol×K	957.41	Joback Method
cpg	1058.33	J/mol×K	993.31	Joback Method
cpg	1071.63	J/mol×K	1029.20	Joback Method
cpg	1083.72	J/mol×K	1065.10	Joback Method
cpg	1094.64	J/mol×K	1100.99	Joback Method
cpg	1104.41	J/mol×K	1136.89	Joback Method
cpg	1113.09	J/mol×K	1172.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380680&Units=SI

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