Sebacic acid, di(2-bromo-4-fluorophenyl) ester

Inchi: InChI=1S/C22H22Br2F2O4/c23-17-13-15(25)9-11-19(17)29-21(27)7-5-3-1-2-4-6-8-22(28
InchiKey: LKJKPGNMXKZYRZ-UHFFFAOYSA-N
Formula: C22H22Br2F2O4
SMILES: O=C(CCCCCCCCC(=O)Oc1ccc(F)cc1Br)Oc1ccc(F)cc1Br
Mol. weight [g/mol]: 548.21

Physical Properties

Property code	Value	Unit	Source
gf	-508.16	kJ/mol	Joback Method
hf	-899.39	kJ/mol	Joback Method
hfus	61.57	kJ/mol	Joback Method
hvap	101.31	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	7.122		Crippen Method
mcvol	326.740	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	3364.00		NIST Webbook
rinpol	3364.00		NIST Webbook
tb	1059.48	K	Joback Method
tc	1299.39	K	Joback Method
tf	705.72	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.41	J/mol×K	1059.48	Joback Method
cpg	979.23	J/mol×K	1099.46	Joback Method
cpg	987.86	J/mol×K	1139.45	Joback Method
cpg	995.33	J/mol×K	1179.43	Joback Method
cpg	1001.72	J/mol×K	1219.42	Joback Method
cpg	1007.09	J/mol×K	1259.40	Joback Method
cpg	1011.49	J/mol×K	1299.39	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=U354564&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