Sebacic acid, di(2-bromo-5-fluorobenzyl) ester

Inchi: InChI=1S/C24H26Br2F2O4/c25-21-11-9-19(27)13-17(21)15-31-23(29)7-5-3-1-2-4-6-8-24
InchiKey: DCEUHFRMKZAXCP-UHFFFAOYSA-N
Formula: C24H26Br2F2O4
SMILES: O=C(CCCCCCCCC(=O)OCc1cc(F)ccc1Br)OCc1cc(F)ccc1Br
Mol. weight [g/mol]: 576.27

Physical Properties

Property code	Value	Unit	Source
gf	-491.32	kJ/mol	Joback Method
hf	-940.67	kJ/mol	Joback Method
hfus	66.75	kJ/mol	Joback Method
hvap	105.77	kJ/mol	Joback Method
log10ws	-9.78		Crippen Method
logp	7.397		Crippen Method
mcvol	354.920	ml/mol	McGowan Method
pc	1293.93	kPa	Joback Method
rinpol	3393.00		NIST Webbook
tb	1105.24	K	Joback Method
tc	1353.12	K	Joback Method
tf	728.26	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.96	J/mol×K	1105.24	Joback Method
cpg	1098.14	J/mol×K	1146.55	Joback Method
cpg	1107.02	J/mol×K	1187.87	Joback Method
cpg	1114.67	J/mol×K	1229.18	Joback Method
cpg	1121.17	J/mol×K	1270.50	Joback Method
cpg	1126.59	J/mol×K	1311.81	Joback Method
cpg	1131.01	J/mol×K	1353.12	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=U380684&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