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

Inchi: InChI=1S/C20H28BrFO4/c1-15(2)14-25-19(23)9-7-5-3-4-6-8-10-20(24)26-18-12-11-16(2

InchiKey: XJVNZYHEQNNONC-UHFFFAOYSA-N

Formula: C20H28BrFO4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 431.34

Physical Properties

Property code	Value	Unit	Source
gf	-440.10	kJ/mol	Joback Method
hf	-907.20	kJ/mol	Joback Method
hfus	51.23	kJ/mol	Joback Method
hvap	87.26	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.814		Crippen Method
mcvol	303.050	ml/mol	McGowan Method
pc	1358.63	kPa	Joback Method
rinpol	2709.00		NIST Webbook
rinpol	2709.00		NIST Webbook
tb	911.21	K	Joback Method
tc	1121.61	K	Joback Method
tf	556.33	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.82	J/mol×K	911.21	Joback Method
cpg	938.91	J/mol×K	946.28	Joback Method
cpg	951.84	J/mol×K	981.34	Joback Method
cpg	963.65	J/mol×K	1016.41	Joback Method
cpg	974.36	J/mol×K	1051.48	Joback Method
cpg	984.01	J/mol×K	1086.55	Joback Method
cpg	992.62	J/mol×K	1121.61	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=U354551&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