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

Inchi: InChI=1S/C20H28BrFO4/c1-2-3-14-25-19(23)10-8-6-4-5-7-9-11-20(24)26-18-13-12-16(2

InchiKey: LDMZQYFZLNFBKO-UHFFFAOYSA-N

Formula: C20H28BrFO4

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

Mol. weight [g/mol]: 431.34

Physical Properties

Property code	Value	Unit	Source
gf	-437.66	kJ/mol	Joback Method
hf	-901.92	kJ/mol	Joback Method
hfus	54.76	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	5.958		Crippen Method
mcvol	303.050	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	2752.00		NIST Webbook
rinpol	2752.00		NIST Webbook
tb	911.65	K	Joback Method
tc	1120.89	K	Joback Method
tf	571.33	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.33	J/mol×K	911.65	Joback Method
cpg	938.37	J/mol×K	946.52	Joback Method
cpg	951.28	J/mol×K	981.40	Joback Method
cpg	963.10	J/mol×K	1016.27	Joback Method
cpg	973.84	J/mol×K	1051.14	Joback Method
cpg	983.54	J/mol×K	1086.02	Joback Method
cpg	992.22	J/mol×K	1120.89	Joback Method

Sources

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=U354552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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