Sebacic acid, 4-bromo-2,6-difluorobenzyl isobutyl ester

Inchi: InChI=1S/C21H29BrF2O4/c1-15(2)13-27-20(25)9-7-5-3-4-6-8-10-21(26)28-14-17-18(23)
InchiKey: KEPYQZZFUCABIW-UHFFFAOYSA-N
Formula: C21H29BrF2O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 463.35

Physical Properties

Property code	Value	Unit	Source
gf	-636.12	kJ/mol	Joback Method
hf	-1135.42	kJ/mol	Joback Method
hfus	56.52	kJ/mol	Joback Method
hvap	89.33	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	6.091		Crippen Method
mcvol	318.910	ml/mol	McGowan Method
pc	1214.90	kPa	Joback Method
rinpol	2734.00		NIST Webbook
rinpol	2734.00		NIST Webbook
tb	938.34	K	Joback Method
tc	1150.08	K	Joback Method
tf	580.71	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.26	J/mol×K	938.34	Joback Method
cpg	1004.23	J/mol×K	973.63	Joback Method
cpg	1016.99	J/mol×K	1008.92	Joback Method
cpg	1028.57	J/mol×K	1044.21	Joback Method
cpg	1039.00	J/mol×K	1079.50	Joback Method
cpg	1048.31	J/mol×K	1114.79	Joback Method
cpg	1056.51	J/mol×K	1150.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380806&Units=SI
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

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