Sebacic acid, 2-bromo-5-fluorobenzyl isobutyl ester

Inchi: InChI=1S/C21H30BrFO4/c1-16(2)14-26-20(24)9-7-5-3-4-6-8-10-21(25)27-15-17-13-18(23

InchiKey: VNYSBCAEGAJWQH-UHFFFAOYSA-N

Formula: C21H30BrFO4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1cc(F)ccc1Br

Mol. weight [g/mol]: 445.36

Physical Properties

Property code	Value	Unit	Source
gf	-431.68	kJ/mol	Joback Method
hf	-927.84	kJ/mol	Joback Method
hfus	53.82	kJ/mol	Joback Method
hvap	89.48	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	5.951		Crippen Method
mcvol	317.140	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook
tb	934.09	K	Joback Method
tc	1146.74	K	Joback Method
tf	567.60	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.21	J/mol×K	934.09	Joback Method
cpg	998.52	J/mol×K	969.53	Joback Method
cpg	1011.62	J/mol×K	1004.97	Joback Method
cpg	1023.54	J/mol×K	1040.42	Joback Method
cpg	1034.33	J/mol×K	1075.86	Joback Method
cpg	1044.00	J/mol×K	1111.30	Joback Method
cpg	1052.61	J/mol×K	1146.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380678&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