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

Inchi: InChI=1S/C21H30BrFO4/c1-2-3-10-15-26-20(24)11-8-6-4-5-7-9-12-21(25)27-19-14-13-17
InchiKey: HEQUFYQQVRHGSN-UHFFFAOYSA-N
Formula: C21H30BrFO4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(F)cc1Br
Mol. weight [g/mol]: 445.36

Physical Properties

Property code	Value	Unit	Source
gf	-429.24	kJ/mol	Joback Method
hf	-922.56	kJ/mol	Joback Method
hfus	57.35	kJ/mol	Joback Method
hvap	89.87	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.348		Crippen Method
mcvol	317.140	ml/mol	McGowan Method
pc	1260.16	kPa	Joback Method
rinpol	2852.00		NIST Webbook
rinpol	2852.00		NIST Webbook
tb	934.53	K	Joback Method
tc	1146.38	K	Joback Method
tf	582.60	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.74	J/mol×K	934.53	Joback Method
cpg	998.04	J/mol×K	969.84	Joback Method
cpg	1011.15	J/mol×K	1005.15	Joback Method
cpg	1023.11	J/mol×K	1040.46	Joback Method
cpg	1033.94	J/mol×K	1075.77	Joback Method
cpg	1043.69	J/mol×K	1111.07	Joback Method
cpg	1052.38	J/mol×K	1146.38	Joback Method

Sources

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=U354553&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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