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

Inchi: InChI=1S/C22H31BrF2O4/c1-2-3-10-13-28-21(26)11-8-6-4-5-7-9-12-22(27)29-16-18-19(
InchiKey: QWBJSFUWNCODBR-UHFFFAOYSA-N
Formula: C22H31BrF2O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 477.38

Physical Properties

Property code	Value	Unit	Source
gf	-625.26	kJ/mol	Joback Method
hf	-1150.78	kJ/mol	Joback Method
hfus	62.63	kJ/mol	Joback Method
hvap	91.94	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	6.625		Crippen Method
mcvol	333.000	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	2879.00		NIST Webbook
rinpol	2879.00		NIST Webbook
tb	961.66	K	Joback Method
tc	1177.36	K	Joback Method
tf	606.98	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.75	J/mol×K	961.66	Joback Method
cpg	1064.03	J/mol×K	997.61	Joback Method
cpg	1077.04	J/mol×K	1033.56	Joback Method
cpg	1088.82	J/mol×K	1069.51	Joback Method
cpg	1099.39	J/mol×K	1105.46	Joback Method
cpg	1108.78	J/mol×K	1141.41	Joback Method
cpg	1117.04	J/mol×K	1177.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380808&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