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

Inchi: InChI=1S/C23H33BrF2O4/c1-2-3-4-11-14-29-22(27)12-9-7-5-6-8-10-13-23(28)30-17-19-
InchiKey: VWLVAGIXLYQLNO-UHFFFAOYSA-N
Formula: C23H33BrF2O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 491.41

Physical Properties

Property code	Value	Unit	Source
gf	-616.84	kJ/mol	Joback Method
hf	-1171.42	kJ/mol	Joback Method
hfus	65.22	kJ/mol	Joback Method
hvap	94.17	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	7.015		Crippen Method
mcvol	347.090	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	2964.00		NIST Webbook
rinpol	2964.00		NIST Webbook
tb	984.54	K	Joback Method
tc	1205.68	K	Joback Method
tf	618.25	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1110.23	J/mol×K	984.54	Joback Method
cpg	1124.83	J/mol×K	1021.40	Joback Method
cpg	1138.07	J/mol×K	1058.25	Joback Method
cpg	1149.98	J/mol×K	1095.11	Joback Method
cpg	1160.61	J/mol×K	1131.97	Joback Method
cpg	1170.00	J/mol×K	1168.82	Joback Method
cpg	1178.18	J/mol×K	1205.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380810&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

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