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

Inchi: InChI=1S/C20H27BrF2O4/c1-2-11-26-19(24)9-7-5-3-4-6-8-10-20(25)27-14-16-17(22)12-
InchiKey: WGCSJQSHTMSYSR-UHFFFAOYSA-N
Formula: C20H27BrF2O4
SMILES: CCCOC(=O)CCCCCCCCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 449.33

Physical Properties

Property code	Value	Unit	Source
gf	-642.10	kJ/mol	Joback Method
hf	-1109.50	kJ/mol	Joback Method
hfus	57.45	kJ/mol	Joback Method
hvap	87.49	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.845		Crippen Method
mcvol	304.820	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2679.00		NIST Webbook
rinpol	2679.00		NIST Webbook
tb	915.90	K	Joback Method
tc	1123.72	K	Joback Method
tf	584.44	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.46	J/mol×K	915.90	Joback Method
cpg	944.14	J/mol×K	950.54	Joback Method
cpg	956.71	J/mol×K	985.17	Joback Method
cpg	968.18	J/mol×K	1019.81	Joback Method
cpg	978.57	J/mol×K	1054.45	Joback Method
cpg	987.91	J/mol×K	1089.09	Joback Method
cpg	996.23	J/mol×K	1123.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380805&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