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

Inchi: InChI=1S/C25H37BrF2O4/c1-2-3-4-5-10-13-16-31-24(29)14-11-8-6-7-9-12-15-25(30)32-
InchiKey: KODFYAXQKCFQHG-UHFFFAOYSA-N
Formula: C25H37BrF2O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 519.46

Physical Properties

Property code	Value	Unit	Source
gf	-600.00	kJ/mol	Joback Method
hf	-1212.70	kJ/mol	Joback Method
hfus	70.40	kJ/mol	Joback Method
hvap	98.62	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	7.795		Crippen Method
mcvol	375.270	ml/mol	McGowan Method
pc	940.37	kPa	Joback Method
rinpol	3147.00		NIST Webbook
rinpol	3147.00		NIST Webbook
tb	1030.30	K	Joback Method
tc	1265.68	K	Joback Method
tf	640.79	K	Joback Method
vc	1.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1232.63	J/mol×K	1030.30	Joback Method
cpg	1247.90	J/mol×K	1069.53	Joback Method
cpg	1261.60	J/mol×K	1108.76	Joback Method
cpg	1273.76	J/mol×K	1147.99	Joback Method
cpg	1284.46	J/mol×K	1187.22	Joback Method
cpg	1293.73	J/mol×K	1226.45	Joback Method
cpg	1301.65	J/mol×K	1265.68	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380812&Units=SI

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