Sebacic acid, di(4-bromo-2,6-difluorobenzyl) ester

Inchi: InChI=1S/C24H24Br2F4O4/c25-15-9-19(27)17(20(28)10-15)13-33-23(31)7-5-3-1-2-4-6-8
InchiKey: URITZRQRAGWNAZ-UHFFFAOYSA-N
Formula: C24H24Br2F4O4
SMILES: O=C(CCCCCCCCC(=O)OCc1c(F)cc(Br)cc1F)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 612.25

Physical Properties

Property code	Value	Unit	Source
gf	-900.20	kJ/mol	Joback Method
hf	-1355.83	kJ/mol	Joback Method
hfus	72.13	kJ/mol	Joback Method
hvap	105.46	kJ/mol	Joback Method
log10ws	-10.44		Crippen Method
logp	7.675		Crippen Method
mcvol	358.460	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
rinpol	3281.00		NIST Webbook
tb	1113.74	K	Joback Method
tc	1365.50	K	Joback Method
tf	754.48	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.99	J/mol×K	1113.74	Joback Method
cpg	1106.43	J/mol×K	1155.70	Joback Method
cpg	1114.43	J/mol×K	1197.66	Joback Method
cpg	1121.04	J/mol×K	1239.62	Joback Method
cpg	1126.34	J/mol×K	1281.58	Joback Method
cpg	1130.38	J/mol×K	1323.54	Joback Method
cpg	1133.23	J/mol×K	1365.50	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=U380814&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