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

Inchi: InChI=1S/C18H12Br2F4O4/c19-9-3-13(21)11(14(22)4-9)7-27-17(25)1-2-18(26)28-8-12-1

InchiKey: WMCHLKVIMCBZLZ-UHFFFAOYSA-N

Formula: C18H12Br2F4O4

SMILES: O=C(CCC(=O)OCc1c(F)cc(Br)cc1F)OCc1c(F)cc(Br)cc1F

Mol. weight [g/mol]: 528.09

Physical Properties

Property code	Value	Unit	Source
gf	-950.72	kJ/mol	Joback Method
hf	-1231.99	kJ/mol	Joback Method
hfus	56.59	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	5.335		Crippen Method
mcvol	273.920	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	2787.00		NIST Webbook
rinpol	2787.00		NIST Webbook
tb	976.46	K	Joback Method
tc	1204.69	K	Joback Method
tf	686.86	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.90	J/mol×K	976.46	Joback Method
cpg	757.16	J/mol×K	1014.50	Joback Method
cpg	764.37	J/mol×K	1052.54	Joback Method
cpg	770.56	J/mol×K	1090.57	Joback Method
cpg	775.77	J/mol×K	1128.61	Joback Method
cpg	780.00	J/mol×K	1166.65	Joback Method
cpg	783.28	J/mol×K	1204.69	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=U381166&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