Succinic acid, 2-bromo-4-fluorophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C17H9BrF6O4/c18-9-5-7(19)1-2-10(9)28-12(26)4-3-11(25)27-6-8-13(20)15(22)
InchiKey: YJWWNPPVCHQUHP-UHFFFAOYSA-N
Formula: C17H9BrF6O4
SMILES: O=C(CCC(=O)Oc1ccc(F)cc1Br)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 471.14

Physical Properties

Property code	Value	Unit	Source
gf	-1372.71	kJ/mol	Joback Method
hf	-1641.37	kJ/mol	Joback Method
hfus	54.48	kJ/mol	Joback Method
hvap	82.47	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	4.713		Crippen Method
mcvol	245.870	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	2370.00		NIST Webbook
tb	890.94	K	Joback Method
tc	1100.04	K	Joback Method
tf	629.49	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.80	J/mol×K	890.94	Joback Method
cpg	688.70	J/mol×K	925.79	Joback Method
cpg	696.68	J/mol×K	960.64	Joback Method
cpg	703.73	J/mol×K	995.49	Joback Method
cpg	709.85	J/mol×K	1030.34	Joback Method
cpg	715.05	J/mol×K	1065.19	Joback Method
cpg	719.33	J/mol×K	1100.04	Joback Method

Sources

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=U358016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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