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

Inchi: InChI=1S/C19H25BrF2O4/c1-2-3-4-5-6-7-10-25-18(23)8-9-19(24)26-13-15-16(21)11-14(
InchiKey: UICXWKOCUJKJRQ-UHFFFAOYSA-N
Formula: C19H25BrF2O4
SMILES: CCCCCCCCOC(=O)CCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 435.30

Physical Properties

Property code	Value	Unit	Source
gf	-650.52	kJ/mol	Joback Method
hf	-1088.86	kJ/mol	Joback Method
hfus	54.86	kJ/mol	Joback Method
hvap	85.26	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.454		Crippen Method
mcvol	290.730	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	2551.00		NIST Webbook
rinpol	2551.00		NIST Webbook
tb	893.02	K	Joback Method
tc	1098.26	K	Joback Method
tf	573.17	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.77	J/mol×K	893.02	Joback Method
cpg	885.16	J/mol×K	927.23	Joback Method
cpg	897.50	J/mol×K	961.43	Joback Method
cpg	908.79	J/mol×K	995.64	Joback Method
cpg	919.07	J/mol×K	1029.85	Joback Method
cpg	928.35	J/mol×K	1064.05	Joback Method
cpg	936.64	J/mol×K	1098.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381159&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