Succinic acid, 4-bromo-2,6-difluorobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H23BrF2O4/c1-4-5-16(11(2)3)25-18(23)7-6-17(22)24-10-13-14(20)8-12(19

InchiKey: BZGOJAFVANSYPP-UHFFFAOYSA-N

Formula: C18H23BrF2O4

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

Mol. weight [g/mol]: 421.27

Physical Properties

Property code	Value	Unit	Source
gf	-663.82	kJ/mol	Joback Method
hf	-1078.78	kJ/mol	Joback Method
hfus	45.22	kJ/mol	Joback Method
hvap	82.26	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	4.919		Crippen Method
mcvol	276.640	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	869.26	K	Joback Method
tc	1075.91	K	Joback Method
tf	531.90	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.88	J/mol×K	869.26	Joback Method
cpg	828.14	J/mol×K	903.70	Joback Method
cpg	840.34	J/mol×K	938.14	Joback Method
cpg	851.49	J/mol×K	972.58	Joback Method
cpg	861.63	J/mol×K	1007.02	Joback Method
cpg	870.76	J/mol×K	1041.47	Joback Method
cpg	878.90	J/mol×K	1075.91	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=U381156&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