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

Inchi: InChI=1S/C18H23BrF2O4/c1-2-3-4-5-6-9-24-17(22)7-8-18(23)25-12-14-15(20)10-13(19)
InchiKey: LKQBGMYUHORXBI-UHFFFAOYSA-N
Formula: C18H23BrF2O4
SMILES: CCCCCCCOC(=O)CCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 421.27

Physical Properties

Property code	Value	Unit	Source
gf	-658.94	kJ/mol	Joback Method
hf	-1068.22	kJ/mol	Joback Method
hfus	52.27	kJ/mol	Joback Method
hvap	83.04	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.064		Crippen Method
mcvol	276.640	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	2449.00		NIST Webbook
rinpol	2449.00		NIST Webbook
tb	870.14	K	Joback Method
tc	1073.62	K	Joback Method
tf	561.90	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.80	J/mol×K	870.14	Joback Method
cpg	826.90	J/mol×K	904.05	Joback Method
cpg	838.99	J/mol×K	937.97	Joback Method
cpg	850.10	J/mol×K	971.88	Joback Method
cpg	860.23	J/mol×K	1005.80	Joback Method
cpg	869.41	J/mol×K	1039.71	Joback Method
cpg	877.66	J/mol×K	1073.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381158&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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