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

Inchi: InChI=1S/C15H17BrF2O4/c1-9(2)7-21-14(19)3-4-15(20)22-8-11-12(17)5-10(16)6-13(11)

InchiKey: KJQLLQLCNCAJRB-UHFFFAOYSA-N

Formula: C15H17BrF2O4

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

Mol. weight [g/mol]: 379.19

Physical Properties

Property code	Value	Unit	Source
gf	-686.64	kJ/mol	Joback Method
hf	-1011.58	kJ/mol	Joback Method
hfus	40.98	kJ/mol	Joback Method
hvap	75.97	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.750		Crippen Method
mcvol	234.370	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
tb	801.06	K	Joback Method
tc	1006.12	K	Joback Method
tf	513.09	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.49	J/mol×K	801.06	Joback Method
cpg	657.73	J/mol×K	835.24	Joback Method
cpg	669.07	J/mol×K	869.41	Joback Method
cpg	679.53	J/mol×K	903.59	Joback Method
cpg	689.11	J/mol×K	937.77	Joback Method
cpg	697.82	J/mol×K	971.95	Joback Method
cpg	705.68	J/mol×K	1006.12	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=U381153&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