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

Inchi: InChI=1S/C14H15BrF2O4/c1-2-5-20-13(18)3-4-14(19)21-8-10-11(16)6-9(15)7-12(10)17/h

InchiKey: ZNVLKTGYAPUZAJ-UHFFFAOYSA-N

Formula: C14H15BrF2O4

SMILES: CCCOC(=O)CCC(=O)OCc1c(F)cc(Br)cc1F

Mol. weight [g/mol]: 365.17

Physical Properties

Property code	Value	Unit	Source
gf	-692.62	kJ/mol	Joback Method
hf	-985.66	kJ/mol	Joback Method
hfus	41.91	kJ/mol	Joback Method
hvap	74.13	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.504		Crippen Method
mcvol	220.280	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	2059.00		NIST Webbook
rinpol	2059.00		NIST Webbook
tb	778.62	K	Joback Method
tc	982.21	K	Joback Method
tf	516.82	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.52	J/mol×K	778.62	Joback Method
cpg	602.21	J/mol×K	812.55	Joback Method
cpg	613.08	J/mol×K	846.48	Joback Method
cpg	623.14	J/mol×K	880.42	Joback Method
cpg	632.39	J/mol×K	914.35	Joback Method
cpg	640.85	J/mol×K	948.28	Joback Method
cpg	648.51	J/mol×K	982.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381152&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