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

Inchi: InChI=1S/C15H17BrF2O4/c1-2-3-6-21-14(19)4-5-15(20)22-9-11-12(17)7-10(16)8-13(11)
InchiKey: VXVCSVKUOJUFAG-UHFFFAOYSA-N
Formula: C15H17BrF2O4
SMILES: CCCCOC(=O)CCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 379.19

Physical Properties

Property code	Value	Unit	Source
gf	-684.20	kJ/mol	Joback Method
hf	-1006.30	kJ/mol	Joback Method
hfus	44.50	kJ/mol	Joback Method
hvap	76.36	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	3.894		Crippen Method
mcvol	234.370	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2154.00		NIST Webbook
rinpol	2154.00		NIST Webbook
tb	801.50	K	Joback Method
tc	1004.10	K	Joback Method
tf	528.09	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.91	J/mol×K	801.50	Joback Method
cpg	657.00	J/mol×K	835.27	Joback Method
cpg	668.23	J/mol×K	869.03	Joback Method
cpg	678.61	J/mol×K	902.80	Joback Method
cpg	688.14	J/mol×K	936.57	Joback Method
cpg	696.84	J/mol×K	970.33	Joback Method
cpg	704.71	J/mol×K	1004.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381154&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