Succinic acid, 3,4-difluorobenzyl isobutyl ester

Inchi: InChI=1S/C15H18F2O4/c1-10(2)8-20-14(18)5-6-15(19)21-9-11-3-4-12(16)13(17)7-11/h3
InchiKey: LKCQCAYLURSECG-UHFFFAOYSA-N
Formula: C15H18F2O4
SMILES: CC(C)COC(=O)CCC(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 300.30

Physical Properties

Property code	Value	Unit	Source
gf	-691.33	kJ/mol	Joback Method
hf	-1026.44	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	68.87	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.987		Crippen Method
mcvol	216.870	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
tb	729.92	K	Joback Method
tc	923.67	K	Joback Method
tf	440.77	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.93	J/mol×K	729.92	Joback Method
cpg	622.70	J/mol×K	762.21	Joback Method
cpg	635.61	J/mol×K	794.50	Joback Method
cpg	647.69	J/mol×K	826.80	Joback Method
cpg	658.93	J/mol×K	859.09	Joback Method
cpg	669.34	J/mol×K	891.38	Joback Method
cpg	678.92	J/mol×K	923.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381741&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