Succinic acid, isobutyl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C15H17F3O4/c1-9(2)7-21-13(19)5-6-14(20)22-8-10-11(16)3-4-12(17)15(10)18

InchiKey: COOJTBMBXUIZDM-UHFFFAOYSA-N

Formula: C15H17F3O4

SMILES: CC(C)COC(=O)CCC(=O)OCc1c(F)ccc(F)c1F

Mol. weight [g/mol]: 318.29

Physical Properties

Property code	Value	Unit	Source
gf	-895.77	kJ/mol	Joback Method
hf	-1234.02	kJ/mol	Joback Method
hfus	38.77	kJ/mol	Joback Method
hvap	68.72	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.127		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
tb	734.17	K	Joback Method
tc	922.85	K	Joback Method
tf	453.88	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.82	J/mol×K	734.17	Joback Method
cpg	628.99	J/mol×K	765.62	Joback Method
cpg	641.37	J/mol×K	797.06	Joback Method
cpg	652.96	J/mol×K	828.51	Joback Method
cpg	663.76	J/mol×K	859.95	Joback Method
cpg	673.78	J/mol×K	891.40	Joback Method
cpg	683.01	J/mol×K	922.85	Joback Method

Sources

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=U381174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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