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

Inchi: InChI=1S/C13H13F3O4/c1-2-19-11(17)5-6-12(18)20-7-8-9(14)3-4-10(15)13(8)16/h3-4H,2

InchiKey: MAHVDTPUSDIIAW-UHFFFAOYSA-N

Formula: C13H13F3O4

SMILES: CCOC(=O)CCC(=O)OCc1c(F)ccc(F)c1F

Mol. weight [g/mol]: 290.24

Physical Properties

Property code	Value	Unit	Source
gf	-910.17	kJ/mol	Joback Method
hf	-1187.46	kJ/mol	Joback Method
hfus	37.11	kJ/mol	Joback Method
hvap	64.66	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.490		Crippen Method
mcvol	190.460	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook
tb	688.85	K	Joback Method
tc	876.71	K	Joback Method
tf	446.34	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.51	J/mol×K	688.85	Joback Method
cpg	521.49	J/mol×K	720.16	Joback Method
cpg	532.79	J/mol×K	751.47	Joback Method
cpg	543.44	J/mol×K	782.78	Joback Method
cpg	553.40	J/mol×K	814.09	Joback Method
cpg	562.70	J/mol×K	845.40	Joback Method
cpg	571.32	J/mol×K	876.71	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=U381173&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