Succinic acid, 2-chloro-6-fluorobenzyl ethyl ester

Inchi: InChI=1S/C13H14ClFO4/c1-2-18-12(16)6-7-13(17)19-8-9-10(14)4-3-5-11(9)15/h3-5H,2,6
InchiKey: XHJYSCAYZYMIIO-UHFFFAOYSA-N
Formula: C13H14ClFO4
SMILES: CCOC(=O)CCC(=O)OCc1c(F)cccc1Cl
Mol. weight [g/mol]: 288.70

Physical Properties

Property code	Value	Unit	Source
gf	-522.85	kJ/mol	Joback Method
hf	-799.51	kJ/mol	Joback Method
hfus	35.54	kJ/mol	Joback Method
hvap	70.01	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.866		Crippen Method
mcvol	199.160	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1904.00		NIST Webbook
rinpol	1904.00		NIST Webbook
tb	722.76	K	Joback Method
tc	927.65	K	Joback Method
tf	462.56	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.75	J/mol×K	722.76	Joback Method
cpg	531.96	J/mol×K	756.91	Joback Method
cpg	543.37	J/mol×K	791.06	Joback Method
cpg	553.98	J/mol×K	825.20	Joback Method
cpg	563.78	J/mol×K	859.35	Joback Method
cpg	572.79	J/mol×K	893.50	Joback Method
cpg	581.01	J/mol×K	927.65	Joback Method

Sources

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=U380857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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