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

Inchi: InChI=1S/C14H16ClFO4/c1-2-8-19-13(17)6-7-14(18)20-9-10-11(15)4-3-5-12(10)16/h3-5

InchiKey: PVBHFGDMFYMYNB-UHFFFAOYSA-N

Formula: C14H16ClFO4

SMILES: CCCOC(=O)CCC(=O)OCc1c(F)cccc1Cl

Mol. weight [g/mol]: 302.73

Physical Properties

Property code	Value	Unit	Source
gf	-514.43	kJ/mol	Joback Method
hf	-820.15	kJ/mol	Joback Method
hfus	38.13	kJ/mol	Joback Method
hvap	72.24	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.256		Crippen Method
mcvol	213.250	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	2016.00		NIST Webbook
rinpol	2016.00		NIST Webbook
tb	745.64	K	Joback Method
tc	948.52	K	Joback Method
tf	473.83	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.64	J/mol×K	745.64	Joback Method
cpg	585.31	J/mol×K	779.45	Joback Method
cpg	597.13	J/mol×K	813.27	Joback Method
cpg	608.11	J/mol×K	847.08	Joback Method
cpg	618.26	J/mol×K	880.89	Joback Method
cpg	627.57	J/mol×K	914.70	Joback Method
cpg	636.05	J/mol×K	948.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380858&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