Succinic acid, 2-chloro-6-fluorophenyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C15H16ClFO5/c16-11-4-1-5-12(17)15(11)22-14(19)7-6-13(18)21-9-10-3-2-8-20

InchiKey: XALIYFWWLKGVLV-UHFFFAOYSA-N

Formula: C15H16ClFO5

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)OCC1CCCO1

Mol. weight [g/mol]: 330.74

Physical Properties

Property code	Value	Unit	Source
gf	-555.58	kJ/mol	Joback Method
hf	-912.31	kJ/mol	Joback Method
hfus	42.63	kJ/mol	Joback Method
hvap	79.23	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.887		Crippen Method
mcvol	222.350	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2347.00		NIST Webbook
rinpol	2347.00		NIST Webbook
tb	810.75	K	Joback Method
tc	1031.30	K	Joback Method
tf	522.57	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.95	J/mol×K	810.75	Joback Method
cpg	659.14	J/mol×K	847.51	Joback Method
cpg	671.18	J/mol×K	884.27	Joback Method
cpg	682.09	J/mol×K	921.02	Joback Method
cpg	691.89	J/mol×K	957.78	Joback Method
cpg	700.58	J/mol×K	994.54	Joback Method
cpg	708.20	J/mol×K	1031.30	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=U390721&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