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

Inchi: InChI=1S/C15H16ClFO4/c16-11-6-3-7-12(17)15(11)21-14(19)9-8-13(18)20-10-4-1-2-5-1(

InchiKey: ZJFBZICHEGVITF-UHFFFAOYSA-N

Formula: C15H16ClFO4

SMILES: O=C(CCC(=O)OC1CCCC1)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 314.74

Physical Properties

Property code	Value	Unit	Source
gf	-469.46	kJ/mol	Joback Method
hf	-780.31	kJ/mol	Joback Method
hfus	34.65	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.650		Crippen Method
mcvol	216.480	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	2194.00		NIST Webbook
rinpol	2194.00		NIST Webbook
tb	783.80	K	Joback Method
tc	1005.84	K	Joback Method
tf	496.00	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.22	J/mol×K	783.80	Joback Method
cpg	630.26	J/mol×K	820.81	Joback Method
cpg	643.15	J/mol×K	857.81	Joback Method
cpg	654.90	J/mol×K	894.82	Joback Method
cpg	665.53	J/mol×K	931.83	Joback Method
cpg	675.07	J/mol×K	968.83	Joback Method
cpg	683.53	J/mol×K	1005.84	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=U391378&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