Succinic acid, 2-chloro-6-fluorophenyl adamant-2-yl ester

Inchi: InChI=1S/C20H22ClFO4/c21-15-2-1-3-16(22)20(15)26-18(24)5-4-17(23)25-19-13-7-11-6

InchiKey: JBWAFCHEPBJEMM-UHFFFAOYSA-N

Formula: C20H22ClFO4

SMILES: O=C(CCC(=O)OC1C2CC3CC(C2)CC1C3)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 380.84

Physical Properties

Property code	Value	Unit	Source
gf	-309.18	kJ/mol	Joback Method
hf	-772.43	kJ/mol	Joback Method
hfus	48.12	kJ/mol	Joback Method
hvap	84.89	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.533		Crippen Method
mcvol	265.210	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	2861.00		NIST Webbook
rinpol	2861.00		NIST Webbook
tb	898.07	K	Joback Method
tc	1124.58	K	Joback Method
tf	583.27	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.61	J/mol×K	898.07	Joback Method
cpg	887.23	J/mol×K	935.82	Joback Method
cpg	901.71	J/mol×K	973.57	Joback Method
cpg	915.16	J/mol×K	1011.33	Joback Method
cpg	927.68	J/mol×K	1049.08	Joback Method
cpg	939.35	J/mol×K	1086.83	Joback Method
cpg	950.28	J/mol×K	1124.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391346&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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