

Succinic acid, 2-chloro-6-fluorophenyl 2-methoxy-5-methylphenyl ester

Inchi:	InChI=1S/C18H16ClFO5/c1-11-6-7-14(23-2)15(10-11)24-16(21)8-9-17(22)25-18-12(19)4
InchiKey:	IBDLMKJTEGDJNL-UHFFFAOYSA-N
Formula:	C18H16ClFO5
SMILES:	COc1ccc(C)cc1OC(=O)CCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]:	366.77

Physical Properties

Property code	Value	Unit	Source
gf	-492.60	kJ/mol	Joback Method
hf	-821.34	kJ/mol	Joback Method
hfus	42.94	kJ/mol	Joback Method
hvap	87.15	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.087		Crippen Method
mvol	251.720	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	896.22	K	Joback Method
tc	1121.70	K	Joback Method
tf	592.60	K	Joback Method
vc	0.961	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.05	J/mol×K	896.22	Joback Method
cpg	731.17	J/mol×K	933.80	Joback Method
cpg	741.00	J/mol×K	971.38	Joback Method
cpg	749.55	J/mol×K	1008.96	Joback Method
cpg	756.81	J/mol×K	1046.54	Joback Method
cpg	762.78	J/mol×K	1084.12	Joback Method
cpg	767.44	J/mol×K	1121.70	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=U390963&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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