

Succinic acid, 2-chloro-6-fluorophenyl 4-chloro-2-methoxyphenyl ester

Inchi:	InChI=1S/C17H13Cl2FO5/c1-23-14-9-10(18)5-6-13(14)24-15(21)7-8-16(22)25-17-11(19)
InchiKey:	WPGGTBUUDUQPNT-UHFFFAOYSA-N
Formula:	C17H13Cl2FO5
SMILES:	COc1cc(Cl)ccc1OC(=O)CCC(=O)Oc1c(F)ccc1Cl
Mol. weight [g/mol]:	387.19

Physical Properties

Property code	Value	Unit	Source
gf	-512.95	kJ/mol	Joback Method
hf	-816.44	kJ/mol	Joback Method
hfus	44.55	kJ/mol	Joback Method
hvap	89.31	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.432		Crippen Method
mcvol	249.870	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook
tb	910.77	K	Joback Method
tc	1141.30	K	Joback Method
tf	611.25	K	Joback Method
vc	0.954	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.97	J/mol×K	910.77	Joback Method
cpg	693.57	J/mol×K	949.19	Joback Method
cpg	701.90	J/mol×K	987.61	Joback Method
cpg	708.96	J/mol×K	1026.04	Joback Method
cpg	714.74	J/mol×K	1064.46	Joback Method
cpg	719.24	J/mol×K	1102.88	Joback Method
cpg	722.45	J/mol×K	1141.30	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=U390941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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