

Succinic acid, 3,5-difluorophenyl 3,4-dimethylphenyl ester

Inchi: InChI=1S/C18H16F2O4/c1-11-3-4-15(7-12(11)2)23-17(21)5-6-18(22)24-16-9-13(19)8-14
InchiKey: ITDPUHQDIHWVHJ-UHFFFAOYSA-N
Formula: C18H16F2O4
SMILES: Cc1ccc(OC(=O)CCC(=O)Oc2cc(F)cc(F)c2)cc1C
Mol. weight [g/mol]: 334.31

Physical Properties

Property code	Value	Unit	Source
gf	-570.48	kJ/mol	Joback Method
hf	-869.49	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	79.54	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	3.873		Crippen Method
mcvol	235.380	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook
tb	835.64	K	Joback Method
tc	1051.92	K	Joback Method
tf	541.04	K	Joback Method
vc	0.911	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.41	J/mol×K	835.64	Joback Method
cpg	692.00	J/mol×K	871.69	Joback Method
cpg	703.48	J/mol×K	907.73	Joback Method
cpg	713.87	J/mol×K	943.78	Joback Method
cpg	723.19	J/mol×K	979.83	Joback Method
cpg	731.43	J/mol×K	1015.87	Joback Method
cpg	738.62	J/mol×K	1051.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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