Succinic acid, 3,5-difluorophenyl 3-fluorophenyl ester

Inchi: InChI=1S/C16H11F3O4/c17-10-2-1-3-13(7-10)22-15(20)4-5-16(21)23-14-8-11(18)6-12(1

InchiKey: WWXAXERVYPFYIC-UHFFFAOYSA-N

Formula: C16H11F3O4

SMILES: O=C(CCC(=O)Oc1cc(F)cc(F)c1)Oc1cccc(F)c1

Mol. weight [g/mol]: 324.25

Physical Properties

Property code	Value	Unit	Source
gf	-772.50	kJ/mol	Joback Method
hf	-1012.85	kJ/mol	Joback Method
hfus	38.92	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.395		Crippen Method
mcvol	208.970	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	2125.00		NIST Webbook
tb	784.17	K	Joback Method
tc	996.52	K	Joback Method
tf	506.57	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.83	J/mol×K	784.17	Joback Method
cpg	590.46	J/mol×K	819.56	Joback Method
cpg	601.11	J/mol×K	854.95	Joback Method
cpg	610.80	J/mol×K	890.34	Joback Method
cpg	619.54	J/mol×K	925.73	Joback Method
cpg	627.35	J/mol×K	961.12	Joback Method
cpg	634.23	J/mol×K	996.52	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=U358034&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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