

Succinic acid, di(3-fluorophenyl) ester

Inchi: InChI=1S/C16H12F2O4/c17-11-3-1-5-13(9-11)21-15(19)7-8-16(20)22-14-6-2-4-12(18)10
InchiKey: YEJDQOHATKVRNS-UHFFFAOYSA-N
Formula: C16H12F2O4
SMILES: O=C(CCC(=O)Oc1cccc(F)c1)Oc1cccc(F)c1
Mol. weight [g/mol]: 306.26

Physical Properties

Property code	Value	Unit	Source
gf	-568.06	kJ/mol	Joback Method
hf	-805.27	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	73.76	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.256		Crippen Method
mcvol	207.200	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	779.92	K	Joback Method
tc	999.04	K	Joback Method
tf	493.46	K	Joback Method
vc	0.799	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.54	J/mol×K	779.92	Joback Method
cpg	584.77	J/mol×K	816.44	Joback Method
cpg	595.96	J/mol×K	852.96	Joback Method
cpg	606.13	J/mol×K	889.48	Joback Method
cpg	615.29	J/mol×K	926.00	Joback Method
cpg	623.46	J/mol×K	962.52	Joback Method
cpg	630.66	J/mol×K	999.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390343&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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