

Succinic acid, 2-fluorophenyl 10-chlorodecyl ester

Inchi:	InChI=1S/C20H28ClFO4/c21-15-9-5-3-1-2-4-6-10-16-25-19(23)13-14-20(24)26-18-12-8-
InchiKey:	ASLKPPOKKMMMECG-UHFFFAOYSA-N
Formula:	C20H28ClFO4
SMILES:	O=C(CCC(=O)Oc1ccccc1F)OCCCCCCCCCCI
Mol. weight [g/mol]:	386.88

Physical Properties

Property code	Value	Unit	Source
gf	-454.28	kJ/mol	Joback Method
hf	-932.52	kJ/mol	Joback Method
hfus	54.06	kJ/mol	Joback Method
hvap	84.93	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.414		Crippen Method
mvol	297.790	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
rmpol	2798.00		NIST Webbook
rmpol	2798.00		NIST Webbook
tb	877.94	K	Joback Method
tc	1080.11	K	Joback Method
tf	528.93	K	Joback Method
vc	1.163	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.21	J/molxK	877.94	Joback Method
cpg	926.84	J/molxK	911.63	Joback Method
cpg	940.35	J/molxK	945.33	Joback Method
cpg	952.77	J/molxK	979.02	Joback Method
cpg	964.12	J/molxK	1012.72	Joback Method
cpg	974.43	J/molxK	1046.41	Joback Method
cpg	983.73	J/molxK	1080.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390411&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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