

Succinic acid, 2-fluorophenyl geranyl ester

Inchi:	InChI=1S/C20H25FO4/c1-15(2)7-6-8-16(3)13-14-24-19(22)11-12-20(23)25-18-10-5-4-9-
InchiKey:	KUJOBMVTXPEIAA-DTQAZKPQSA-N
Formula:	C20H25FO4
SMILES:	CC(C)=CCCC(C)=CCOC(=O)CCC(=O)Oc1ccccc1F
Mol. weight [g/mol]:	348.41

Physical Properties

Property code	Value	Unit	Source
gf	-299.01	kJ/mol	Joback Method
hf	-701.92	kJ/mol	Joback Method
hfus	47.65	kJ/mol	Joback Method
hvap	80.62	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.747		Crippen Method
mcvol	276.950	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2447.00		NIST Webbook
rinpol	2447.00		NIST Webbook
tb	848.59	K	Joback Method
tc	1055.83	K	Joback Method
tf	460.93	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.27	J/mol×K	848.59	Joback Method
cpg	846.28	J/mol×K	883.13	Joback Method
cpg	860.30	J/mol×K	917.67	Joback Method
cpg	873.37	J/mol×K	952.21	Joback Method
cpg	885.54	J/mol×K	986.75	Joback Method
cpg	896.87	J/mol×K	1021.29	Joback Method
cpg	907.40	J/mol×K	1055.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U391213&Units=SI

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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