

Succinic acid, 2-fluorophenyl 2-ethoxyethyl ester

Inchi:	InChI=1S/C14H17FO5/c1-2-18-9-10-19-13(16)7-8-14(17)20-12-6-4-3-5-11(12)15/h3-6H,1
InchiKey:	DBULLMZCSMUZON-UHFFFAOYSA-N
Formula:	C14H17FO5
SMILES:	CCOCCOC(=O)CCC(=O)Oc1ccccc1F
Mol. weight [g/mol]:	284.28

Physical Properties

Property code	Value	Unit	Source
gf	-597.87	kJ/mol	Joback Method
hf	-925.16	kJ/mol	Joback Method
hfus	35.51	kJ/mol	Joback Method
hvap	69.60	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.091		Crippen Method
mcvol	206.880	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	725.65	K	Joback Method
tc	923.01	K	Joback Method
tf	453.62	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.46	J/molxK	725.65	Joback Method
cpg	587.97	J/molxK	758.54	Joback Method
cpg	600.62	J/molxK	791.44	Joback Method
cpg	612.41	J/molxK	824.33	Joback Method
cpg	623.34	J/molxK	857.22	Joback Method
cpg	633.40	J/molxK	890.11	Joback Method
cpg	642.59	J/molxK	923.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Latest version available from:

<https://www.chemeo.com/cid/120-673-1/Succinic-acid-2-fluorophenyl-2-ethoxyethyl-ester.pdf>

Generated by Cheméo on 2024-04-28 20:06:18.194073022 +0000 UTC m=+16624027.114650337.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.