Succinic acid, 2-fluorophenyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C15H17FO5/c16-12-5-1-2-6-13(12)21-15(18)8-7-14(17)20-10-11-4-3-9-19-11/h

InchiKey: WRUHLFUNFNENEQ-UHFFFAOYSA-N

Formula: C15H17FO5

SMILES: O=C(CCC(=O)Oc1ccccc1F)OCC1CCCO1

Mol. weight [g/mol]: 296.29

Physical Properties

Property code	Value	Unit	Source
gf	-534.02	kJ/mol	Joback Method
hf	-885.10	kJ/mol	Joback Method
hfus	38.83	kJ/mol	Joback Method
hvap	74.18	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.234		Crippen Method
mcvol	210.110	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	2174.00		NIST Webbook
tb	768.34	K	Joback Method
tc	984.98	K	Joback Method
tf	480.13	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.25	J/mol×K	768.34	Joback Method
cpg	636.87	J/mol×K	804.45	Joback Method
cpg	650.33	J/mol×K	840.55	Joback Method
cpg	662.66	J/mol×K	876.66	Joback Method
cpg	673.88	J/mol×K	912.77	Joback Method
cpg	684.02	J/mol×K	948.87	Joback Method
cpg	693.09	J/mol×K	984.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390719&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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