Succinic acid, cyclohexylmethyl 3-fluorophenyl ester

Inchi: InChI=1S/C17H21FO4/c18-14-7-4-8-15(11-14)22-17(20)10-9-16(19)21-12-13-5-2-1-3-6-1

InchiKey: GNGPJCZYNFYNJH-UHFFFAOYSA-N

Formula: C17H21FO4

SMILES: O=C(CCC(=O)Oc1cccc(F)c1)OCC1CCCCC1

Mol. weight [g/mol]: 308.34

Physical Properties

Property code	Value	Unit	Source
gf	-443.16	kJ/mol	Joback Method
hf	-800.54	kJ/mol	Joback Method
hfus	33.93	kJ/mol	Joback Method
hvap	74.30	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.635		Crippen Method
mcvol	232.420	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	791.42	K	Joback Method
tc	1009.64	K	Joback Method
tf	472.58	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.12	J/mol×K	791.42	Joback Method
cpg	722.45	J/mol×K	827.79	Joback Method
cpg	737.45	J/mol×K	864.16	Joback Method
cpg	751.12	J/mol×K	900.53	Joback Method
cpg	763.51	J/mol×K	936.90	Joback Method
cpg	774.62	J/mol×K	973.27	Joback Method
cpg	784.49	J/mol×K	1009.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390332&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
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