Succinic acid, phenethyl 3-fluorophenyl ester

Inchi: InChI=1S/C18H17FO4/c19-15-7-4-8-16(13-15)23-18(21)10-9-17(20)22-12-11-14-5-2-1-3
InchiKey: LXIKUPAQABPHSL-UHFFFAOYSA-N
Formula: C18H17FO4
SMILES: O=C(CCC(=O)Oc1cccc(F)c1)OCCc1ccccc1
Mol. weight [g/mol]: 316.32

Physical Properties

Property code	Value	Unit	Source
gf	-346.78	kJ/mol	Joback Method
hf	-638.97	kJ/mol	Joback Method
hfus	38.72	kJ/mol	Joback Method
hvap	78.37	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.297		Crippen Method
mcvol	233.610	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2404.00		NIST Webbook
tb	821.43	K	Joback Method
tc	1042.32	K	Joback Method
tf	502.89	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.72	J/mol×K	821.43	Joback Method
cpg	689.10	J/mol×K	858.25	Joback Method
cpg	701.31	J/mol×K	895.06	Joback Method
cpg	712.39	J/mol×K	931.88	Joback Method
cpg	722.36	J/mol×K	968.69	Joback Method
cpg	731.25	J/mol×K	1005.51	Joback Method
cpg	739.09	J/mol×K	1042.32	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=U358004&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