Succinic acid, 4-fluorophenethyl isobutyl ester

Inchi: InChI=1S/C16H21FO4/c1-12(2)11-21-16(19)8-7-15(18)20-10-9-13-3-5-14(17)6-4-13/h3-6
InchiKey: PURGHIDVFFXMQI-UHFFFAOYSA-N
Formula: C16H21FO4
SMILES: CC(C)COC(=O)CCC(=O)OCCc1ccc(F)cc1
Mol. weight [g/mol]: 296.33

Physical Properties

Property code	Value	Unit	Source
gf	-478.47	kJ/mol	Joback Method
hf	-839.50	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	71.26	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.891		Crippen Method
mcvol	229.190	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
tb	748.55	K	Joback Method
tc	946.59	K	Joback Method
tf	438.93	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.73	J/mol×K	748.55	Joback Method
cpg	671.50	J/mol×K	781.56	Joback Method
cpg	685.32	J/mol×K	814.56	Joback Method
cpg	698.20	J/mol×K	847.57	Joback Method
cpg	710.16	J/mol×K	880.57	Joback Method
cpg	721.20	J/mol×K	913.58	Joback Method
cpg	731.34	J/mol×K	946.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381296&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