Succinic acid, 4-fluorobenzyl propyl ester

Inchi: InChI=1S/C14H17FO4/c1-2-9-18-13(16)7-8-14(17)19-10-11-3-5-12(15)6-4-11/h3-6H,2,7-
InchiKey: DFCAXFSRTWCJAJ-UHFFFAOYSA-N
Formula: C14H17FO4
SMILES: CCCOC(=O)CCC(=O)OCc1ccc(F)cc1
Mol. weight [g/mol]: 268.28

Physical Properties

Property code	Value	Unit	Source
gf	-492.87	kJ/mol	Joback Method
hf	-792.94	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	67.19	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.602		Crippen Method
mcvol	201.010	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1831.00		NIST Webbook
rinpol	1831.00		NIST Webbook
tb	703.23	K	Joback Method
tc	901.55	K	Joback Method
tf	431.39	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.87	J/mol×K	703.23	Joback Method
cpg	561.65	J/mol×K	736.28	Joback Method
cpg	574.59	J/mol×K	769.34	Joback Method
cpg	586.70	J/mol×K	802.39	Joback Method
cpg	597.99	J/mol×K	835.45	Joback Method
cpg	608.45	J/mol×K	868.50	Joback Method
cpg	618.11	J/mol×K	901.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381668&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

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