Succinic acid, 2-fluorophenyl 3-methylbutyl ester

Inchi: InChI=1S/C15H19FO4/c1-11(2)9-10-19-14(17)7-8-15(18)20-13-6-4-3-5-12(13)16/h3-6,11
InchiKey: ZCMRKBOLILUOTD-UHFFFAOYSA-N
Formula: C15H19FO4
SMILES: CC(C)CCOC(=O)CCC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 282.31

Physical Properties

Property code	Value	Unit	Source
gf	-486.89	kJ/mol	Joback Method
hf	-818.86	kJ/mol	Joback Method
hfus	33.39	kJ/mol	Joback Method
hvap	69.03	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.101		Crippen Method
mcvol	215.100	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
tb	725.67	K	Joback Method
tc	925.21	K	Joback Method
tf	427.66	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.99	J/mol×K	725.67	Joback Method
cpg	616.42	J/mol×K	758.93	Joback Method
cpg	629.93	J/mol×K	792.18	Joback Method
cpg	642.53	J/mol×K	825.44	Joback Method
cpg	654.25	J/mol×K	858.69	Joback Method
cpg	665.08	J/mol×K	891.95	Joback Method
cpg	675.03	J/mol×K	925.21	Joback Method

Sources

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=U370962&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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