Succinic acid, 3-methylbut-2-en-1-yl 2-fluorophenyl ester

Inchi: InChI=1S/C15H17FO4/c1-11(2)9-10-19-14(17)7-8-15(18)20-13-6-4-3-5-12(13)16/h3-6,9H
InchiKey: RTZRQEWKVLNBJX-UHFFFAOYSA-N
Formula: C15H17FO4
SMILES: CC(C)=CCOC(=O)CCC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 280.29

Physical Properties

Property code	Value	Unit	Source
gf	-412.78	kJ/mol	Joback Method
hf	-706.15	kJ/mol	Joback Method
hfus	35.80	kJ/mol	Joback Method
hvap	69.46	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.021		Crippen Method
mcvol	210.800	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tb	730.15	K	Joback Method
tc	935.65	K	Joback Method
tf	423.62	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.17	J/mol×K	730.15	Joback Method
cpg	590.97	J/mol×K	764.40	Joback Method
cpg	603.88	J/mol×K	798.65	Joback Method
cpg	615.92	J/mol×K	832.90	Joback Method
cpg	627.10	J/mol×K	867.15	Joback Method
cpg	637.46	J/mol×K	901.40	Joback Method
cpg	647.02	J/mol×K	935.65	Joback Method

Sources

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=U390306&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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