

Succinic acid, 1-(2-fluorophenyl)ethyl isobutyl ester

Inchi:	InChI=1S/C16H21FO4/c1-11(2)10-20-15(18)8-9-16(19)21-12(3)13-6-4-5-7-14(13)17/h4-7
InchiKey:	WEPADLQLFJDXNZ-UHFFFAOYSA-N
Formula:	C16H21FO4
SMILES:	CC(C)COC(=O)CCC(=O)OC(C)c1ccccc1F
Mol. weight [g/mol]:	296.33

Physical Properties

Property code	Value	Unit	Source
gf	-480.91	kJ/mol	Joback Method
hf	-844.78	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	70.87	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.409		Crippen Method
mvol	229.190	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	748.11	K	Joback Method
tc	948.92	K	Joback Method
tf	423.93	K	Joback Method
vc	0.877	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.27	J/mol×K	748.11	Joback Method
cpg	672.26	J/mol×K	781.58	Joback Method
cpg	686.26	J/mol×K	815.05	Joback Method
cpg	699.29	J/mol×K	848.52	Joback Method
cpg	711.36	J/mol×K	881.98	Joback Method
cpg	722.47	J/mol×K	915.45	Joback Method
cpg	732.65	J/mol×K	948.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U381391&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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