

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

Inchi:	InChI=1S/C17H23FO4/c1-12(2)11-21-16(19)9-6-10-17(20)22-13(3)14-7-4-5-8-15(14)18/H
InchiKey:	SJPABTCTLDLPHX-UHFFFAOYSA-N
Formula:	C17H23FO4
SMILES:	CC(C)COC(=O)CCCC(=O)OC(C)c1ccccc1F
Mol. weight [g/mol]:	310.36

Physical Properties

Property code	Value	Unit	Source
gf	-472.49	kJ/mol	Joback Method
hf	-865.42	kJ/mol	Joback Method
hfus	35.05	kJ/mol	Joback Method
hvap	73.09	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.799		Crippen Method
mcvol	243.280	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinqol	2046.00		NIST Webbook
tb	770.99	K	Joback Method
tc	970.54	K	Joback Method
tf	435.20	K	Joback Method
vc	0.933	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.08	J/mol×K	770.99	Joback Method
cpg	728.35	J/mol×K	804.25	Joback Method
cpg	742.60	J/mol×K	837.51	Joback Method
cpg	755.84	J/mol×K	870.76	Joback Method
cpg	768.09	J/mol×K	904.02	Joback Method
cpg	779.35	J/mol×K	937.28	Joback Method
cpg	789.66	J/mol×K	970.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377072&Units=SI
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

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
mccvol:	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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