

Glutaric acid, 2-fluorophenyl 4-fluoro-2-methoxyphenyl ester

Inchi:	InChI=1S/C18H16F2O5/c1-23-16-11-12(19)9-10-15(16)25-18(22)8-4-7-17(21)24-14-6-3-
InchiKey:	UHAAIANXBUILCB-UHFFFAOYSA-N
Formula:	C18H16F2O5
SMILES:	COc1cc(F)ccc1OC(=O)CCCC(=O)Oc1ccccc1F
Mol. weight [g/mol]:	350.31

Physical Properties

Property code	Value	Unit	Source
gf	-665.85	kJ/mol	Joback Method
hf	-990.24	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	81.29	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.655		Crippen Method
mcvol	241.250	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	2434.00		NIST Webbook
rinpol	2434.00		NIST Webbook
tb	853.08	K	Joback Method
tc	1067.96	K	Joback Method
tf	550.75	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.09	J/mol×K	853.08	Joback Method
cpg	719.24	J/mol×K	888.89	Joback Method
cpg	730.22	J/mol×K	924.71	Joback Method
cpg	740.02	J/mol×K	960.52	Joback Method
cpg	748.65	J/mol×K	996.33	Joback Method
cpg	756.12	J/mol×K	1032.14	Joback Method
cpg	762.42	J/mol×K	1067.96	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=U393445&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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