Glutaric acid, di(3-fluorophenyl) ester

Inchi: InChI=1S/C17H14F2O4/c18-12-4-1-6-14(10-12)22-16(20)8-3-9-17(21)23-15-7-2-5-13(19
InchiKey: VRDCLTDCFLVVNE-UHFFFAOYSA-N
Formula: C17H14F2O4
SMILES: O=C(CCCC(=O)Oc1cccc(F)c1)Oc1cccc(F)c1
Mol. weight [g/mol]: 320.29

Physical Properties

Property code	Value	Unit	Source
gf	-559.64	kJ/mol	Joback Method
hf	-825.91	kJ/mol	Joback Method
hfus	38.82	kJ/mol	Joback Method
hvap	75.99	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.646		Crippen Method
mcvol	221.290	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	2328.00		NIST Webbook
rinpol	2328.00		NIST Webbook
tb	802.80	K	Joback Method
tc	1019.43	K	Joback Method
tf	504.73	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.78	J/mol×K	802.80	Joback Method
cpg	639.31	J/mol×K	838.91	Joback Method
cpg	650.76	J/mol×K	875.01	Joback Method
cpg	661.16	J/mol×K	911.12	Joback Method
cpg	670.54	J/mol×K	947.22	Joback Method
cpg	678.90	J/mol×K	983.33	Joback Method
cpg	686.27	J/mol×K	1019.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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