Glutaric acid, 2-fluorophenyl 2-nitrophenyl ester

Inchi: InChI=1S/C17H14FNO6/c18-12-6-1-3-8-14(12)24-16(20)10-5-11-17(21)25-15-9-4-2-7-13

InchiKey: NKVCWIXGDJJFHD-UHFFFAOYSA-N

Formula: C17H14FNO6

SMILES: O=C(CCCC(=O)Oc1ccccc1[N+](=O)[O-])Oc1ccccc1F

Mol. weight [g/mol]: 347.29

Physical Properties

Property code	Value	Unit	Source
gf	-329.28	kJ/mol	Joback Method
hf	-640.56	kJ/mol	Joback Method
hfus	47.10	kJ/mol	Joback Method
hvap	93.40	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	3.415		Crippen Method
mcvol	236.940	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook
tb	955.37	K	Joback Method
tc	1197.81	K	Joback Method
tf	647.75	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.36	J/mol×K	955.37	Joback Method
cpg	720.68	J/mol×K	995.78	Joback Method
cpg	728.72	J/mol×K	1036.18	Joback Method
cpg	735.50	J/mol×K	1076.59	Joback Method
cpg	741.06	J/mol×K	1117.00	Joback Method
cpg	745.43	J/mol×K	1157.40	Joback Method
cpg	748.65	J/mol×K	1197.81	Joback Method

Sources

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=U393319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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