Glutaric acid, 2-fluorophenyl 3-nitrobenzyl ester

Inchi: InChI=1S/C18H16FNO6/c19-15-7-1-2-8-16(15)26-18(22)10-4-9-17(21)25-12-13-5-3-6-14

InchiKey: FNBBSSTYTXOSTI-UHFFFAOYSA-N

Formula: C18H16FNO6

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCc1cccc([N+](=O)[O-])c1

Mol. weight [g/mol]: 361.32

Physical Properties

Property code	Value	Unit	Source
gf	-320.86	kJ/mol	Joback Method
hf	-661.20	kJ/mol	Joback Method
hfus	49.69	kJ/mol	Joback Method
hvap	95.62	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	3.553		Crippen Method
mcvol	251.030	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
tb	978.25	K	Joback Method
tc	1219.04	K	Joback Method
tf	659.02	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.90	J/mol×K	978.25	Joback Method
cpg	777.32	J/mol×K	1018.38	Joback Method
cpg	785.43	J/mol×K	1058.51	Joback Method
cpg	792.26	J/mol×K	1098.64	Joback Method
cpg	797.86	J/mol×K	1138.77	Joback Method
cpg	802.26	J/mol×K	1178.91	Joback Method
cpg	805.51	J/mol×K	1219.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393356&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