Glutaric acid, 2-chloro-6-fluorophenyl 3-nitrobenzyl ester

Inchi: InChI=1S/C18H15ClFNO6/c19-14-6-2-7-15(20)18(14)27-17(23)9-3-8-16(22)26-11-12-4-1
InchiKey: YGFDSOFEVKGBLX-UHFFFAOYSA-N
Formula: C18H15ClFNO6
SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 395.77

Physical Properties

Property code	Value	Unit	Source
gf	-342.42	kJ/mol	Joback Method
hf	-688.41	kJ/mol	Joback Method
hfus	53.50	kJ/mol	Joback Method
hvap	100.67	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.206		Crippen Method
mcvol	263.270	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	3037.00		NIST Webbook
rinpol	3037.00		NIST Webbook
tb	1020.66	K	Joback Method
tc	1266.05	K	Joback Method
tf	701.46	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.90	J/mol×K	1020.66	Joback Method
cpg	790.78	J/mol×K	1061.56	Joback Method
cpg	797.32	J/mol×K	1102.46	Joback Method
cpg	802.56	J/mol×K	1143.36	Joback Method
cpg	806.54	J/mol×K	1184.25	Joback Method
cpg	809.30	J/mol×K	1225.15	Joback Method
cpg	810.86	J/mol×K	1266.05	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=U393359&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