Glutaric acid, cyclohexylmethyl 2-nitrophenyl ester

Inchi: InChI=1S/C18H23NO6/c20-17(24-13-14-7-2-1-3-8-14)11-6-12-18(21)25-16-10-5-4-9-15(
InchiKey: IQVDFPJMDOUWMK-UHFFFAOYSA-N
Formula: C18H23NO6
SMILES: O=C(CCCC(=O)Oc1ccccc1[N+](=O)[O-])OCC1CCCCC1
Mol. weight [g/mol]: 349.38

Physical Properties

Property code	Value	Unit	Source
gf	-204.38	kJ/mol	Joback Method
hf	-635.83	kJ/mol	Joback Method
hfus	44.80	kJ/mol	Joback Method
hvap	93.93	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	3.794		Crippen Method
mcvol	262.160	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	2781.00		NIST Webbook
rinpol	2781.00		NIST Webbook
tb	966.87	K	Joback Method
tc	1208.73	K	Joback Method
tf	626.87	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.54	J/mol×K	966.87	Joback Method
cpg	874.81	J/mol×K	1007.18	Joback Method
cpg	885.45	J/mol×K	1047.49	Joback Method
cpg	894.51	J/mol×K	1087.80	Joback Method
cpg	902.02	J/mol×K	1128.11	Joback Method
cpg	908.02	J/mol×K	1168.42	Joback Method
cpg	912.56	J/mol×K	1208.73	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=U393320&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