Glutaric acid, 2-(4-nitrophenoxy)ethyl pentyl ester

Inchi: InChI=1S/C18H25NO7/c1-2-3-4-12-25-17(20)6-5-7-18(21)26-14-13-24-16-10-8-15(9-11-
InchiKey: SCQAQBABNNRQBE-UHFFFAOYSA-N
Formula: C18H25NO7
SMILES: CCCCCOC(=O)CCCC(=O)OCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 367.39

Physical Properties

Property code	Value	Unit	Source
gf	-333.83	kJ/mol	Joback Method
hf	-822.37	kJ/mol	Joback Method
hfus	54.15	kJ/mol	Joback Method
hvap	95.91	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.420		Crippen Method
mcvol	278.890	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	2911.00		NIST Webbook
rinpol	2911.00		NIST Webbook
tb	969.74	K	Joback Method
tc	1193.76	K	Joback Method
tf	641.72	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.72	J/mol×K	969.74	Joback Method
cpg	908.24	J/mol×K	1007.08	Joback Method
cpg	918.36	J/mol×K	1044.41	Joback Method
cpg	927.08	J/mol×K	1081.75	Joback Method
cpg	934.43	J/mol×K	1119.08	Joback Method
cpg	940.40	J/mol×K	1156.42	Joback Method
cpg	945.03	J/mol×K	1193.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376796&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

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