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

Inchi: InChI=1S/C16H21NO7/c1-2-10-23-15(18)4-3-5-16(19)24-12-11-22-14-8-6-13(7-9-14)17(
InchiKey: OLCCNUZEXAOKGU-UHFFFAOYSA-N
Formula: C16H21NO7
SMILES: CCCOC(=O)CCCC(=O)OCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 339.34

Physical Properties

Property code	Value	Unit	Source
gf	-350.67	kJ/mol	Joback Method
hf	-781.09	kJ/mol	Joback Method
hfus	48.97	kJ/mol	Joback Method
hvap	91.46	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.640		Crippen Method
mcvol	250.710	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	2706.00		NIST Webbook
rinpol	2706.00		NIST Webbook
tb	923.98	K	Joback Method
tc	1146.57	K	Joback Method
tf	619.18	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.04	J/mol×K	923.98	Joback Method
cpg	792.43	J/mol×K	961.08	Joback Method
cpg	802.52	J/mol×K	998.18	Joback Method
cpg	811.33	J/mol×K	1035.27	Joback Method
cpg	818.86	J/mol×K	1072.37	Joback Method
cpg	825.11	J/mol×K	1109.47	Joback Method
cpg	830.08	J/mol×K	1146.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376793&Units=SI

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