Glutaric acid, hex-4-yn-3-yl 4-nitrophenyl ester

Inchi: InChI=1S/C17H19NO6/c1-3-6-14(4-2)23-16(19)7-5-8-17(20)24-15-11-9-13(10-12-15)18(
InchiKey: PWZDBBCJLPUDEZ-UHFFFAOYSA-N
Formula: C17H19NO6
SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 333.34

Physical Properties

Property code	Value	Unit	Source
gf	-36.89	kJ/mol	Joback Method
hf	-402.49	kJ/mol	Joback Method
hfus	49.97	kJ/mol	Joback Method
hvap	93.04	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.016		Crippen Method
mcvol	250.330	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	2548.00		NIST Webbook
rinpol	2548.00		NIST Webbook
tb	933.00	K	Joback Method
tc	1171.84	K	Joback Method
tf	699.32	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.89	J/mol×K	933.00	Joback Method
cpg	768.39	J/mol×K	972.81	Joback Method
cpg	778.58	J/mol×K	1012.61	Joback Method
cpg	787.48	J/mol×K	1052.42	Joback Method
cpg	795.12	J/mol×K	1092.23	Joback Method
cpg	801.52	J/mol×K	1132.03	Joback Method
cpg	806.71	J/mol×K	1171.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391974&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