Glutaric acid, 3-methyl-4-nitrobenzyl propyl ester

Inchi: InChI=1S/C16H21NO6/c1-3-9-22-15(18)5-4-6-16(19)23-11-13-7-8-14(17(20)21)12(2)10-
InchiKey: GZEZASAMHVCOHR-UHFFFAOYSA-N
Formula: C16H21NO6
SMILES: CCCOC(=O)CCCC(=O)OCc1ccc([N+](=O)[O-])c(C)c1
Mol. weight [g/mol]: 323.34

Physical Properties

Property code	Value	Unit	Source
gf	-255.30	kJ/mol	Joback Method
hf	-660.34	kJ/mol	Joback Method
hfus	47.39	kJ/mol	Joback Method
hvap	89.71	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.070		Crippen Method
mcvol	244.840	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	906.54	K	Joback Method
tc	1129.81	K	Joback Method
tf	609.47	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.56	J/mol×K	906.54	Joback Method
cpg	765.56	J/mol×K	943.75	Joback Method
cpg	776.37	J/mol×K	980.96	Joback Method
cpg	786.01	J/mol×K	1018.18	Joback Method
cpg	794.48	J/mol×K	1055.39	Joback Method
cpg	801.81	J/mol×K	1092.60	Joback Method
cpg	808.00	J/mol×K	1129.81	Joback Method

Sources

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=U376846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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