Glutaric acid, 3-methylbut-2-yl 4-nitrophenyl ester

Inchi: InChI=1S/C16H21NO6/c1-11(2)12(3)22-15(18)5-4-6-16(19)23-14-9-7-13(8-10-14)17(20)
InchiKey: KCPWFBTZCGGCBM-UHFFFAOYSA-N
Formula: C16H21NO6
SMILES: CC(C)C(C)OC(=O)CCCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 323.34

Physical Properties

Property code	Value	Unit	Source
gf	-250.55	kJ/mol	Joback Method
hf	-659.43	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	88.27	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.258		Crippen Method
mcvol	244.840	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2391.00		NIST Webbook
rinpol	2391.00		NIST Webbook
tb	900.68	K	Joback Method
tc	1128.23	K	Joback Method
tf	566.95	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.02	J/mol×K	900.68	Joback Method
cpg	768.32	J/mol×K	938.61	Joback Method
cpg	779.35	J/mol×K	976.53	Joback Method
cpg	789.16	J/mol×K	1014.46	Joback Method
cpg	797.75	J/mol×K	1052.38	Joback Method
cpg	805.16	J/mol×K	1090.31	Joback Method
cpg	811.41	J/mol×K	1128.23	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=U391970&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