Glutaric acid, 3-methylbut-2-en-1-yl 2-nitrophenyl ester

Inchi: InChI=1S/C16H19NO6/c1-12(2)10-11-22-15(18)8-5-9-16(19)23-14-7-4-3-6-13(14)17(20)
InchiKey: XAEUBDUVEDRBMZ-UHFFFAOYSA-N
Formula: C16H19NO6
SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 321.33

Physical Properties

Property code	Value	Unit	Source
gf	-174.00	kJ/mol	Joback Method
hf	-541.44	kJ/mol	Joback Method
hfus	46.67	kJ/mol	Joback Method
hvap	89.09	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.180		Crippen Method
mcvol	240.540	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	2447.00		NIST Webbook
rinpol	2447.00		NIST Webbook
tb	905.60	K	Joback Method
tc	1135.73	K	Joback Method
tf	577.91	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.42	J/mol×K	905.60	Joback Method
cpg	738.27	J/mol×K	943.95	Joback Method
cpg	749.03	J/mol×K	982.31	Joback Method
cpg	758.73	J/mol×K	1020.66	Joback Method
cpg	767.42	J/mol×K	1059.02	Joback Method
cpg	775.13	J/mol×K	1097.37	Joback Method
cpg	781.91	J/mol×K	1135.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393315&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