Glutaric acid, isobutyl 2-nitrophenyl ester

Inchi: InChI=1S/C15H19NO6/c1-11(2)10-21-14(17)8-5-9-15(18)22-13-7-4-3-6-12(13)16(19)20/
InchiKey: ASIGKQGJCJUZHU-UHFFFAOYSA-N
Formula: C15H19NO6
SMILES: CC(C)COC(=O)CCCC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 309.31

Physical Properties

Property code	Value	Unit	Source
gf	-256.53	kJ/mol	Joback Method
hf	-633.51	kJ/mol	Joback Method
hfus	41.67	kJ/mol	Joback Method
hvap	86.44	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	2.870		Crippen Method
mcvol	230.750	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	2329.00		NIST Webbook
rinpol	2329.00		NIST Webbook
tb	878.24	K	Joback Method
tc	1104.68	K	Joback Method
tf	570.68	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.81	J/mol×K	878.24	Joback Method
cpg	710.85	J/mol×K	915.98	Joback Method
cpg	721.71	J/mol×K	953.72	Joback Method
cpg	731.40	J/mol×K	991.46	Joback Method
cpg	739.95	J/mol×K	1029.20	Joback Method
cpg	747.37	J/mol×K	1066.94	Joback Method
cpg	753.69	J/mol×K	1104.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358754&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