Glutaric acid, ethyl 3-nitro-4-methoxybenzyl ester

Inchi: InChI=1S/C15H19NO7/c1-3-22-14(17)5-4-6-15(18)23-10-11-7-8-13(21-2)12(9-11)16(19)
InchiKey: ACRNHEIDONDDKO-UHFFFAOYSA-N
Formula: C15H19NO7
SMILES: CCOC(=O)CCCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 325.31

Physical Properties

Property code	Value	Unit	Source
gf	-368.72	kJ/mol	Joback Method
hf	-771.92	kJ/mol	Joback Method
hfus	45.99	kJ/mol	Joback Method
hvap	89.90	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.380		Crippen Method
mcvol	236.620	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	2546.00		NIST Webbook
tb	906.08	K	Joback Method
tc	1129.95	K	Joback Method
tf	620.43	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.65	J/mol×K	906.08	Joback Method
cpg	733.82	J/mol×K	943.39	Joback Method
cpg	743.73	J/mol×K	980.70	Joback Method
cpg	752.37	J/mol×K	1018.02	Joback Method
cpg	759.74	J/mol×K	1055.33	Joback Method
cpg	765.82	J/mol×K	1092.64	Joback Method
cpg	770.63	J/mol×K	1129.95	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377038&Units=SI

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