Glutaric acid, 3,5-dinitrobenzyl ethyl ester

Inchi: InChI=1S/C14H16N2O8/c1-2-23-13(17)4-3-5-14(18)24-9-10-6-11(15(19)20)8-12(7-10)16
InchiKey: KNSZIBLOECSYTK-UHFFFAOYSA-N
Formula: C14H16N2O8
SMILES: CCOC(=O)CCCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 340.29

Physical Properties

Property code	Value	Unit	Source
gf	-236.59	kJ/mol	Joback Method
hf	-629.82	kJ/mol	Joback Method
hfus	53.57	kJ/mol	Joback Method
hvap	101.85	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	2.280		Crippen Method
mcvol	234.080	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	2608.00		NIST Webbook
tb	1012.62	K	Joback Method
tc	1258.17	K	Joback Method
tf	730.54	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.17	J/mol×K	1012.62	Joback Method
cpg	734.95	J/mol×K	1053.54	Joback Method
cpg	741.40	J/mol×K	1094.47	Joback Method
cpg	746.54	J/mol×K	1135.39	Joback Method
cpg	750.40	J/mol×K	1176.32	Joback Method
cpg	752.97	J/mol×K	1217.24	Joback Method
cpg	754.29	J/mol×K	1258.17	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=U376867&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