Glutaric acid, 3,5-dinitro-2-methylbenzyl ethyl ester

Inchi: InChI=1S/C15H18N2O8/c1-3-24-14(18)5-4-6-15(19)25-9-11-7-12(16(20)21)8-13(10(11)2

InchiKey: FNVVFMXMUDQUMN-UHFFFAOYSA-N

Formula: C15H18N2O8

SMILES: CCOC(=O)CCCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1C

Mol. weight [g/mol]: 354.31

Physical Properties

Property code	Value	Unit	Source
gf	-237.80	kJ/mol	Joback Method
hf	-661.93	kJ/mol	Joback Method
hfus	55.78	kJ/mol	Joback Method
hvap	104.74	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	2.588		Crippen Method
mcvol	248.170	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	2681.00		NIST Webbook
tb	1040.48	K	Joback Method
tc	1286.37	K	Joback Method
tf	754.33	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.00	J/mol×K	1040.48	Joback Method
cpg	789.64	J/mol×K	1081.46	Joback Method
cpg	795.86	J/mol×K	1122.44	Joback Method
cpg	800.67	J/mol×K	1163.43	Joback Method
cpg	804.09	J/mol×K	1204.41	Joback Method
cpg	806.13	J/mol×K	1245.39	Joback Method
cpg	806.81	J/mol×K	1286.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377015&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