Glutaric acid, 3,5-dinitrobenzyl isobutyl ester

Inchi: InChI=1S/C16H20N2O8/c1-11(2)9-25-15(19)4-3-5-16(20)26-10-12-6-13(17(21)22)8-14(7
InchiKey: WCAZMUOLLKEYJY-UHFFFAOYSA-N
Formula: C16H20N2O8
SMILES: CC(C)COC(=O)CCCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 368.34

Physical Properties

Property code	Value	Unit	Source
gf	-222.19	kJ/mol	Joback Method
hf	-676.38	kJ/mol	Joback Method
hfus	55.23	kJ/mol	Joback Method
hvap	105.92	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	2.916		Crippen Method
mcvol	262.260	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	2756.00		NIST Webbook
rinpol	2756.00		NIST Webbook
tb	1057.94	K	Joback Method
tc	1305.16	K	Joback Method
tf	738.08	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.71	J/mol×K	1057.94	Joback Method
cpg	849.53	J/mol×K	1099.14	Joback Method
cpg	855.90	J/mol×K	1140.35	Joback Method
cpg	860.86	J/mol×K	1181.55	Joback Method
cpg	864.43	J/mol×K	1222.76	Joback Method
cpg	866.63	J/mol×K	1263.96	Joback Method
cpg	867.50	J/mol×K	1305.16	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=U376869&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