Glutaric acid, 3,5-dinitrobenzyl pentyl ester

Inchi: InChI=1S/C17H22N2O8/c1-2-3-4-8-26-16(20)6-5-7-17(21)27-12-13-9-14(18(22)23)11-15

InchiKey: BELHHHGMUYYKLS-UHFFFAOYSA-N

Formula: C17H22N2O8

SMILES: CCCCCOC(=O)CCCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1

Mol. weight [g/mol]: 382.37

Physical Properties

Property code	Value	Unit	Source
gf	-211.33	kJ/mol	Joback Method
hf	-691.74	kJ/mol	Joback Method
hfus	61.34	kJ/mol	Joback Method
hvap	108.53	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	3.450		Crippen Method
mcvol	276.350	ml/mol	McGowan Method
pc	1689.34	kPa	Joback Method
rinpol	2902.00		NIST Webbook
rinpol	2902.00		NIST Webbook
tb	1081.26	K	Joback Method
tc	1328.28	K	Joback Method
tf	764.35	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.22	J/mol×K	1081.26	Joback Method
cpg	907.10	J/mol×K	1122.43	Joback Method
cpg	913.51	J/mol×K	1163.60	Joback Method
cpg	918.50	J/mol×K	1204.77	Joback Method
cpg	922.10	J/mol×K	1245.94	Joback Method
cpg	924.33	J/mol×K	1287.11	Joback Method
cpg	925.24	J/mol×K	1328.28	Joback Method

Sources

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=U376871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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