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

Inchi: InChI=1S/C21H30N2O8/c1-3-4-5-6-7-8-12-30-20(24)10-9-11-21(25)31-15-17-13-18(22(2

InchiKey: PPSIJDSAEHQFTG-UHFFFAOYSA-N

Formula: C21H30N2O8

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

Mol. weight [g/mol]: 438.47

Physical Properties

Property code	Value	Unit	Source
gf	-187.28	kJ/mol	Joback Method
hf	-785.77	kJ/mol	Joback Method
hfus	71.32	kJ/mol	Joback Method
hvap	118.10	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	4.929		Crippen Method
mcvol	332.710	ml/mol	McGowan Method
pc	1246.85	kPa	Joback Method
rinpol	3274.00		NIST Webbook
tb	1177.76	K	Joback Method
tc	1442.94	K	Joback Method
tf	821.95	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1131.79	J/mol×K	1177.76	Joback Method
cpg	1139.10	J/mol×K	1221.96	Joback Method
cpg	1144.56	J/mol×K	1266.15	Joback Method
cpg	1148.22	J/mol×K	1310.35	Joback Method
cpg	1150.14	J/mol×K	1354.55	Joback Method
cpg	1150.35	J/mol×K	1398.75	Joback Method
cpg	1148.93	J/mol×K	1442.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377022&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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