Glutaric acid, 3,5-dinitro-2-methylbenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C20H28N2O8/c1-5-7-18(13(2)3)30-20(24)9-6-8-19(23)29-12-15-10-16(21(25)2
InchiKey: PFTWUUYEJXKLEA-UHFFFAOYSA-N
Formula: C20H28N2O8
SMILES: CCCC(OC(=O)CCCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1C)C(C)C
Mol. weight [g/mol]: 424.44

Physical Properties

Property code	Value	Unit	Source
gf	-200.58	kJ/mol	Joback Method
hf	-775.69	kJ/mol	Joback Method
hfus	61.68	kJ/mol	Joback Method
hvap	115.09	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	4.393		Crippen Method
mcvol	318.620	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	3016.00		NIST Webbook
rinpol	3016.00		NIST Webbook
tb	1154.00	K	Joback Method
tc	1412.97	K	Joback Method
tf	780.68	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.75	J/mol×K	1154.00	Joback Method
cpg	1079.88	J/mol×K	1197.16	Joback Method
cpg	1085.22	J/mol×K	1240.32	Joback Method
cpg	1088.82	J/mol×K	1283.48	Joback Method
cpg	1090.71	J/mol×K	1326.65	Joback Method
cpg	1090.94	J/mol×K	1369.81	Joback Method
cpg	1089.55	J/mol×K	1412.97	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=U377019&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