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

Inchi: InChI=1S/C20H28N2O8/c1-3-4-5-6-7-11-29-19(23)9-8-10-20(24)30-14-16-12-17(21(25)2
InchiKey: OPDMKEVVHZIADM-UHFFFAOYSA-N
Formula: C20H28N2O8
SMILES: CCCCCCCOC(=O)CCCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1C
Mol. weight [g/mol]: 424.44

Physical Properties

Property code	Value	Unit	Source
gf	-195.70	kJ/mol	Joback Method
hf	-765.13	kJ/mol	Joback Method
hfus	68.73	kJ/mol	Joback Method
hvap	115.87	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	4.539		Crippen Method
mcvol	318.620	ml/mol	McGowan Method
pc	1335.88	kPa	Joback Method
rinpol	3173.00		NIST Webbook
tb	1154.88	K	Joback Method
tc	1413.95	K	Joback Method
tf	810.68	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.68	J/mol×K	1154.88	Joback Method
cpg	1080.09	J/mol×K	1198.06	Joback Method
cpg	1085.75	J/mol×K	1241.24	Joback Method
cpg	1089.71	J/mol×K	1284.41	Joback Method
cpg	1092.00	J/mol×K	1327.59	Joback Method
cpg	1092.66	J/mol×K	1370.77	Joback Method
cpg	1091.75	J/mol×K	1413.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377021&Units=SI

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