Glutaric acid, 3,5-dinitrobenzyl heptyl ester

Inchi: InChI=1S/C19H26N2O8/c1-2-3-4-5-6-10-28-18(22)8-7-9-19(23)29-14-15-11-16(20(24)25
InchiKey: MFZUQHPZOWODPV-UHFFFAOYSA-N
Formula: C19H26N2O8
SMILES: CCCCCCCOC(=O)CCCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 410.42

Physical Properties

Property code	Value	Unit	Source
gf	-194.49	kJ/mol	Joback Method
hf	-733.02	kJ/mol	Joback Method
hfus	66.53	kJ/mol	Joback Method
hvap	112.98	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	4.230		Crippen Method
mcvol	304.530	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
rinpol	3105.00		NIST Webbook
rinpol	3105.00		NIST Webbook
tb	1127.02	K	Joback Method
tc	1380.16	K	Joback Method
tf	786.89	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.07	J/mol×K	1127.02	Joback Method
cpg	1023.91	J/mol×K	1169.21	Joback Method
cpg	1030.17	J/mol×K	1211.40	Joback Method
cpg	1034.89	J/mol×K	1253.59	Joback Method
cpg	1038.12	J/mol×K	1295.78	Joback Method
cpg	1039.90	J/mol×K	1337.97	Joback Method
cpg	1040.28	J/mol×K	1380.16	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=U376874&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