Glutaric acid, 3,5-dinitrobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C19H26N2O8/c1-4-6-17(13(2)3)29-19(23)8-5-7-18(22)28-12-14-9-15(20(24)25
InchiKey: HAOHFYIQMYGJCU-UHFFFAOYSA-N
Formula: C19H26N2O8
SMILES: CCCC(OC(=O)CCCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1)C(C)C
Mol. weight [g/mol]: 410.42

Physical Properties

Property code	Value	Unit	Source
gf	-199.37	kJ/mol	Joback Method
hf	-743.58	kJ/mol	Joback Method
hfus	59.48	kJ/mol	Joback Method
hvap	112.21	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	4.084		Crippen Method
mcvol	304.530	ml/mol	McGowan Method
pc	1469.10	kPa	Joback Method
rinpol	2947.00		NIST Webbook
rinpol	2947.00		NIST Webbook
tb	1126.14	K	Joback Method
tc	1380.18	K	Joback Method
tf	756.89	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.32	J/mol×K	1126.14	Joback Method
cpg	1023.93	J/mol×K	1168.48	Joback Method
cpg	1029.91	J/mol×K	1210.82	Joback Method
cpg	1034.30	J/mol×K	1253.16	Joback Method
cpg	1037.16	J/mol×K	1295.50	Joback Method
cpg	1038.52	J/mol×K	1337.84	Joback Method
cpg	1038.44	J/mol×K	1380.18	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=U376872&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