Glutaric acid, 3,5-dinitrobenzyl hexyl ester

Inchi: InChI=1S/C18H24N2O8/c1-2-3-4-5-9-27-17(21)7-6-8-18(22)28-13-14-10-15(19(23)24)12
InchiKey: IDCDOONUCVEWKW-UHFFFAOYSA-N
Formula: C18H24N2O8
SMILES: CCCCCCOC(=O)CCCC(=O)OCc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 396.39

Physical Properties

Property code	Value	Unit	Source
gf	-202.91	kJ/mol	Joback Method
hf	-712.38	kJ/mol	Joback Method
hfus	63.93	kJ/mol	Joback Method
hvap	110.76	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	3.840		Crippen Method
mcvol	290.440	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	2995.00		NIST Webbook
tb	1104.14	K	Joback Method
tc	1353.67	K	Joback Method
tf	775.62	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.46	J/mol×K	1104.14	Joback Method
cpg	965.33	J/mol×K	1145.73	Joback Method
cpg	971.67	J/mol×K	1187.32	Joback Method
cpg	976.54	J/mol×K	1228.91	Joback Method
cpg	979.97	J/mol×K	1270.49	Joback Method
cpg	982.01	J/mol×K	1312.08	Joback Method
cpg	982.68	J/mol×K	1353.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376873&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

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