Glutaric acid, di(3-methyl-2-nitrobenzyl) ester

Inchi: InChI=1S/C21H22N2O8/c1-14-6-3-8-16(20(14)22(26)27)12-30-18(24)10-5-11-19(25)31-1
InchiKey: ZMVREQDZQFMVDZ-UHFFFAOYSA-N
Formula: C21H22N2O8
SMILES: Cc1cccc(COC(=O)CCCC(=O)OCc2cccc(C)c2[N+](=O)[O-])c1[N+](=O)[O-]
Mol. weight [g/mol]: 430.41

Physical Properties

Property code	Value	Unit	Source
gf	-84.50	kJ/mol	Joback Method
hf	-560.71	kJ/mol	Joback Method
hfus	64.97	kJ/mol	Joback Method
hvap	121.03	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	4.077		Crippen Method
mcvol	308.950	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	3452.00		NIST Webbook
tb	1209.42	K	Joback Method
tc	1482.07	K	Joback Method
tf	860.89	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.71	J/mol×K	1209.42	Joback Method
cpg	1007.68	J/mol×K	1254.86	Joback Method
cpg	1009.89	J/mol×K	1300.30	Joback Method
cpg	1010.40	J/mol×K	1345.75	Joback Method
cpg	1009.27	J/mol×K	1391.19	Joback Method
cpg	1006.54	J/mol×K	1436.63	Joback Method
cpg	1002.29	J/mol×K	1482.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376743&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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