Glutaric acid, pentyl 3-methoxy-4-nitrobenzyl ester

Inchi: InChI=1S/C18H25NO7/c1-3-4-5-11-25-17(20)7-6-8-18(21)26-13-14-9-10-15(19(22)23)16

InchiKey: NYBSFXJZUROIIY-UHFFFAOYSA-N

Formula: C18H25NO7

SMILES: CCCCCOC(=O)CCCC(=O)OCc1ccc([N+](=O)[O-])c(OC)c1

Mol. weight [g/mol]: 367.39

Physical Properties

Property code	Value	Unit	Source
gf	-343.46	kJ/mol	Joback Method
hf	-833.84	kJ/mol	Joback Method
hfus	53.76	kJ/mol	Joback Method
hvap	96.58	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.550		Crippen Method
mcvol	278.890	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	2852.00		NIST Webbook
rinpol	2852.00		NIST Webbook
tb	974.72	K	Joback Method
tc	1199.63	K	Joback Method
tf	654.24	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.30	J/mol×K	974.72	Joback Method
cpg	906.67	J/mol×K	1012.21	Joback Method
cpg	916.61	J/mol×K	1049.69	Joback Method
cpg	925.11	J/mol×K	1087.18	Joback Method
cpg	932.18	J/mol×K	1124.66	Joback Method
cpg	937.84	J/mol×K	1162.15	Joback Method
cpg	942.07	J/mol×K	1199.63	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=U376892&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