Glutaric acid, dodecyl 3-nitrophenethyl ester

Inchi: InChI=1S/C25H39NO6/c1-2-3-4-5-6-7-8-9-10-11-19-31-24(27)16-13-17-25(28)32-20-18-
InchiKey: NSIZCEVJYQOZPJ-UHFFFAOYSA-N
Formula: C25H39NO6
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OCCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 449.58

Physical Properties

Property code	Value	Unit	Source
gf	-169.89	kJ/mol	Joback Method
hf	-834.63	kJ/mol	Joback Method
hfus	71.09	kJ/mol	Joback Method
hvap	109.08	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	6.315		Crippen Method
mcvol	371.650	ml/mol	McGowan Method
pc	977.78	kPa	Joback Method
rinpol	3444.00		NIST Webbook
tb	1107.48	K	Joback Method
tc	1359.81	K	Joback Method
tf	698.38	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.28	J/mol×K	1107.48	Joback Method
cpg	1304.53	J/mol×K	1149.54	Joback Method
cpg	1316.00	J/mol×K	1191.59	Joback Method
cpg	1325.78	J/mol×K	1233.65	Joback Method
cpg	1333.94	J/mol×K	1275.70	Joback Method
cpg	1340.56	J/mol×K	1317.76	Joback Method
cpg	1345.73	J/mol×K	1359.81	Joback Method

Sources

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=U376755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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