Glutaric acid, tridec-2-yn-1-yl 3-nitrobenzyl ester

Inchi: InChI=1S/C25H35NO6/c1-2-3-4-5-6-7-8-9-10-11-12-19-31-24(27)17-14-18-25(28)32-21-
InchiKey: ZUMYMELFMRDGJQ-UHFFFAOYSA-N
Formula: C25H35NO6
SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 445.55

Physical Properties

Property code	Value	Unit	Source
gf	32.91	kJ/mol	Joback Method
hf	-562.33	kJ/mol	Joback Method
hfus	74.22	kJ/mol	Joback Method
hvap	111.24	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	5.886		Crippen Method
mcvol	363.050	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	3468.00		NIST Webbook
rinpol	3468.00		NIST Webbook
tb	1116.48	K	Joback Method
tc	1367.26	K	Joback Method
tf	804.48	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.18	J/mol×K	1116.48	Joback Method
cpg	1242.06	J/mol×K	1158.28	Joback Method
cpg	1252.26	J/mol×K	1200.07	Joback Method
cpg	1260.87	J/mol×K	1241.87	Joback Method
cpg	1267.94	J/mol×K	1283.66	Joback Method
cpg	1273.55	J/mol×K	1325.46	Joback Method
cpg	1277.76	J/mol×K	1367.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393366&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