Glutaric acid, 3-nitro-4-methoxybenzyl octyl ester

Inchi: InChI=1S/C21H31NO7/c1-3-4-5-6-7-8-14-28-20(23)10-9-11-21(24)29-16-17-12-13-19(27

InchiKey: CGLBHBPLWHMTBS-UHFFFAOYSA-N

Formula: C21H31NO7

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

Mol. weight [g/mol]: 409.47

Physical Properties

Property code	Value	Unit	Source
gf	-318.20	kJ/mol	Joback Method
hf	-895.76	kJ/mol	Joback Method
hfus	61.53	kJ/mol	Joback Method
hvap	103.25	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	4.721		Crippen Method
mcvol	321.160	ml/mol	McGowan Method
pc	1234.61	kPa	Joback Method
rinpol	3150.00		NIST Webbook
tb	1043.36	K	Joback Method
tc	1277.49	K	Joback Method
tf	688.05	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.55	J/mol×K	1043.36	Joback Method
cpg	1083.93	J/mol×K	1082.38	Joback Method
cpg	1093.61	J/mol×K	1121.40	Joback Method
cpg	1101.62	J/mol×K	1160.42	Joback Method
cpg	1107.98	J/mol×K	1199.44	Joback Method
cpg	1112.70	J/mol×K	1238.47	Joback Method
cpg	1115.79	J/mol×K	1277.49	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=U377046&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

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