Glutaric acid, isobutyl 4-methyl-3-nitrobenzyl ester

Inchi: InChI=1S/C17H23NO6/c1-12(2)10-23-16(19)5-4-6-17(20)24-11-14-8-7-13(3)15(9-14)18(

InchiKey: ASUMXMLMGASXGU-UHFFFAOYSA-N

Formula: C17H23NO6

SMILES: Cc1ccc(COC(=O)CCCC(=O)OCC(C)C)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 337.37

Physical Properties

Property code	Value	Unit	Source
gf	-249.32	kJ/mol	Joback Method
hf	-686.26	kJ/mol	Joback Method
hfus	46.46	kJ/mol	Joback Method
hvap	91.55	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.316		Crippen Method
mcvol	258.930	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	2523.00		NIST Webbook
tb	928.98	K	Joback Method
tc	1153.96	K	Joback Method
tf	605.74	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.53	J/mol×K	928.98	Joback Method
cpg	823.74	J/mol×K	966.48	Joback Method
cpg	834.67	J/mol×K	1003.97	Joback Method
cpg	844.36	J/mol×K	1041.47	Joback Method
cpg	852.82	J/mol×K	1078.97	Joback Method
cpg	860.06	J/mol×K	1116.47	Joback Method
cpg	866.11	J/mol×K	1153.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376779&Units=SI

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