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

Inchi: InChI=1S/C17H23NO7/c1-12(2)10-24-16(19)5-4-6-17(20)25-11-13-7-8-15(23-3)14(9-13)

InchiKey: NHGPRDPHPPXHOM-UHFFFAOYSA-N

Formula: C17H23NO7

SMILES: COc1ccc(COC(=O)CCCC(=O)OCC(C)C)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 353.37

Physical Properties

Property code	Value	Unit	Source
gf	-354.32	kJ/mol	Joback Method
hf	-818.48	kJ/mol	Joback Method
hfus	47.65	kJ/mol	Joback Method
hvap	93.96	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.016		Crippen Method
mcvol	264.800	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2699.00		NIST Webbook
tb	951.40	K	Joback Method
tc	1176.90	K	Joback Method
tf	627.97	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.64	J/mol×K	951.40	Joback Method
cpg	849.01	J/mol×K	988.98	Joback Method
cpg	858.97	J/mol×K	1026.57	Joback Method
cpg	867.53	J/mol×K	1064.15	Joback Method
cpg	874.68	J/mol×K	1101.73	Joback Method
cpg	880.42	J/mol×K	1139.31	Joback Method
cpg	884.76	J/mol×K	1176.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377040&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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