Glutaric acid, cyclohexylmethyl 3-nitrobenzyl ester

Inchi: InChI=1S/C19H25NO6/c21-18(25-13-15-6-2-1-3-7-15)10-5-11-19(22)26-14-16-8-4-9-17(
InchiKey: BGZGBVYTBNZDND-UHFFFAOYSA-N
Formula: C19H25NO6
SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 363.40

Physical Properties

Property code	Value	Unit	Source
gf	-195.96	kJ/mol	Joback Method
hf	-656.47	kJ/mol	Joback Method
hfus	47.39	kJ/mol	Joback Method
hvap	96.16	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	3.932		Crippen Method
mcvol	276.250	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	2971.00		NIST Webbook
tb	989.75	K	Joback Method
tc	1230.32	K	Joback Method
tf	638.14	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.07	J/mol×K	989.75	Joback Method
cpg	933.22	J/mol×K	1029.85	Joback Method
cpg	943.73	J/mol×K	1069.94	Joback Method
cpg	952.63	J/mol×K	1110.04	Joback Method
cpg	959.98	J/mol×K	1150.13	Joback Method
cpg	965.82	J/mol×K	1190.23	Joback Method
cpg	970.20	J/mol×K	1230.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393358&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

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