Glutaric acid, ethyl 2-nitro-3-chlorobenzyl ester

Inchi: InChI=1S/C14H16ClNO6/c1-2-21-12(17)7-4-8-13(18)22-9-10-5-3-6-11(15)14(10)16(19)2

InchiKey: LZVRKUINWUQSMV-UHFFFAOYSA-N

Formula: C14H16ClNO6

SMILES: CCOC(=O)CCCC(=O)OCc1cccc(Cl)c1[N+](=O)[O-]

Mol. weight [g/mol]: 329.73

Physical Properties

Property code	Value	Unit	Source
gf	-284.07	kJ/mol	Joback Method
hf	-634.80	kJ/mol	Joback Method
hfus	46.41	kJ/mol	Joback Method
hvap	89.65	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.025		Crippen Method
mcvol	228.900	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
tb	898.21	K	Joback Method
tc	1127.74	K	Joback Method
tf	616.85	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.45	J/mol×K	898.21	Joback Method
cpg	671.81	J/mol×K	936.46	Joback Method
cpg	681.04	J/mol×K	974.72	Joback Method
cpg	689.17	J/mol×K	1012.97	Joback Method
cpg	696.19	J/mol×K	1051.23	Joback Method
cpg	702.12	J/mol×K	1089.48	Joback Method
cpg	706.97	J/mol×K	1127.74	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=U377023&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

Latest version available from:
https://www.chemeo.com/cid/59-830-5/Glutaric-acid-ethyl-2-nitro-3-chlorobenzyl-ester.pdf
Generated by Cheméo on 2024-04-19 21:23:19.710848962 +0000 UTC m=+15851048.631426281.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.