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

Inchi: InChI=1S/C18H24ClNO6/c1-2-3-4-5-12-25-16(21)10-7-11-17(22)26-13-14-8-6-9-15(19)1

InchiKey: DJNVBSFGANFXTC-UHFFFAOYSA-N

Formula: C18H24ClNO6

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

Mol. weight [g/mol]: 385.84

Physical Properties

Property code	Value	Unit	Source
gf	-250.39	kJ/mol	Joback Method
hf	-717.36	kJ/mol	Joback Method
hfus	56.77	kJ/mol	Joback Method
hvap	98.55	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	4.585		Crippen Method
mcvol	285.260	ml/mol	McGowan Method
pc	1504.65	kPa	Joback Method
rinpol	2770.00		NIST Webbook
tb	989.73	K	Joback Method
tc	1218.40	K	Joback Method
tf	661.93	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.82	J/mol×K	989.73	Joback Method
cpg	900.77	J/mol×K	1027.84	Joback Method
cpg	910.43	J/mol×K	1065.95	Joback Method
cpg	918.82	J/mol×K	1104.07	Joback Method
cpg	925.97	J/mol×K	1142.18	Joback Method
cpg	931.90	J/mol×K	1180.29	Joback Method
cpg	936.64	J/mol×K	1218.40	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=U377029&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