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

Inchi: InChI=1S/C16H20ClNO6/c1-11(2)9-23-14(19)7-4-8-15(20)24-10-12-5-3-6-13(17)16(12)1

InchiKey: OUYGRUSVHXNHNT-UHFFFAOYSA-N

Formula: C16H20ClNO6

SMILES: CC(C)COC(=O)CCCC(=O)OCc1cccc(Cl)c1[N+](=O)[O-]

Mol. weight [g/mol]: 357.79

Physical Properties

Property code	Value	Unit	Source
gf	-269.67	kJ/mol	Joback Method
hf	-681.36	kJ/mol	Joback Method
hfus	48.07	kJ/mol	Joback Method
hvap	93.71	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.661		Crippen Method
mcvol	257.080	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2558.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	943.53	K	Joback Method
tc	1173.19	K	Joback Method
tf	624.39	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.82	J/mol×K	943.53	Joback Method
cpg	785.58	J/mol×K	981.81	Joback Method
cpg	795.10	J/mol×K	1020.08	Joback Method
cpg	803.40	J/mol×K	1058.36	Joback Method
cpg	810.50	J/mol×K	1096.64	Joback Method
cpg	816.42	J/mol×K	1134.92	Joback Method
cpg	821.17	J/mol×K	1173.19	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=U377025&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