Glutaric acid, cyclohexylmethyl 3-chlorophenyl ester

Inchi: InChI=1S/C18H23ClO4/c19-15-8-4-9-16(12-15)23-18(21)11-5-10-17(20)22-13-14-6-2-1-3

InchiKey: XFVBAGCVRSYIOY-UHFFFAOYSA-N

Formula: C18H23ClO4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)OCC1CCCCC1

Mol. weight [g/mol]: 338.83

Physical Properties

Property code	Value	Unit	Source
gf	-251.86	kJ/mol	Joback Method
hf	-640.81	kJ/mol	Joback Method
hfus	37.63	kJ/mol	Joback Method
hvap	81.73	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.539		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		NIST Webbook
tb	852.46	K	Joback Method
tc	1078.83	K	Joback Method
tf	513.18	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.42	J/mol×K	852.46	Joback Method
cpg	797.89	J/mol×K	890.19	Joback Method
cpg	811.91	J/mol×K	927.92	Joback Method
cpg	824.52	J/mol×K	965.64	Joback Method
cpg	835.73	J/mol×K	1003.37	Joback Method
cpg	845.59	J/mol×K	1041.10	Joback Method
cpg	854.12	J/mol×K	1078.83	Joback Method
dvisc	0.0006773	Pa×s	513.18	Joback Method

dvisc	0.0003777	Pa×s	569.73	Joback Method
dvisc	0.0002341	Pa×s	626.27	Joback Method
dvisc	0.0001570	Pa×s	682.82	Joback Method
dvisc	0.0001120	Pa×s	739.37	Joback Method
dvisc	0.0000838	Pa×s	795.91	Joback Method
dvisc	0.0000651	Pa×s	852.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390522&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
dvisc:	Dynamic viscosity
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