Glutaric acid, 3-chlorophenyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C19H27ClO4/c1-14(12-19(2,3)4)13-23-17(21)9-6-10-18(22)24-16-8-5-7-15(20)

InchiKey: MQFXDJFFMYHJKL-UHFFFAOYSA-N

Formula: C19H27ClO4

SMILES: CC(COC(=O)CCCC(=O)Oc1cccc(Cl)c1)CC(C)(C)C

Mol. weight [g/mol]: 354.87

Physical Properties

Property code	Value	Unit	Source
gf	-267.49	kJ/mol	Joback Method
hf	-729.80	kJ/mol	Joback Method
hfus	37.45	kJ/mol	Joback Method
hvap	81.84	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	5.031		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
tb	852.12	K	Joback Method
tc	1064.25	K	Joback Method
tf	504.49	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.86	J/mol×K	852.12	Joback Method
cpg	911.97	J/mol×K	1028.89	Joback Method
cpg	901.28	J/mol×K	993.54	Joback Method
cpg	889.57	J/mol×K	958.18	Joback Method
cpg	876.79	J/mol×K	922.83	Joback Method
cpg	862.90	J/mol×K	887.47	Joback Method
cpg	921.68	J/mol×K	1064.25	Joback Method
dvisc	0.0000394	Pa×s	852.12	Joback Method

dvisc	0.0000521	Pa×s	794.18	Joback Method
dvisc	0.0000720	Pa×s	736.24	Joback Method
dvisc	0.0001052	Pa×s	678.30	Joback Method
dvisc	0.0001650	Pa×s	620.37	Joback Method
dvisc	0.0002839	Pa×s	562.43	Joback Method
dvisc	0.0005533	Pa×s	504.49	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=U391536&Units=SI

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