Glutaric acid, 3-chlorophenyl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C18H25ClO5/c1-14(9-11-22-2)10-12-23-17(20)7-4-8-18(21)24-16-6-3-5-15(19)

InchiKey: DNCIVNUWRDWISI-UHFFFAOYSA-N

Formula: C18H25ClO5

SMILES: COCCC(C)CCOC(=O)CCCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 356.84

Physical Properties

Property code	Value	Unit	Source
gf	-383.75	kJ/mol	Joback Method
hf	-832.63	kJ/mol	Joback Method
hfus	43.46	kJ/mol	Joback Method
hvap	83.32	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.022		Crippen Method
mcvol	273.710	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2504.00		NIST Webbook
rinpol	2504.00		NIST Webbook
tb	854.89	K	Joback Method
tc	1061.59	K	Joback Method
tf	513.03	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.98	J/mol×K	854.89	Joback Method
cpg	831.15	J/mol×K	889.34	Joback Method
cpg	844.14	J/mol×K	923.79	Joback Method
cpg	855.96	J/mol×K	958.24	Joback Method
cpg	866.63	J/mol×K	992.69	Joback Method
cpg	876.15	J/mol×K	1027.14	Joback Method
cpg	884.53	J/mol×K	1061.59	Joback Method
dvisc	0.0004669	Pa×s	513.03	Joback Method

dvisc	0.0002575	Pa×s	570.01	Joback Method
dvisc	0.0001582	Pa×s	626.98	Joback Method
dvisc	0.0001054	Pa×s	683.96	Joback Method
dvisc	0.0000748	Pa×s	740.94	Joback Method
dvisc	0.0000557	Pa×s	797.91	Joback Method
dvisc	0.0000432	Pa×s	854.89	Joback Method

Sources

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=U393527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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