Glutaric acid, 3-chlorophenyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C18H25ClO4/c1-12(2)18(13(3)4)23-17(21)10-6-9-16(20)22-15-8-5-7-14(19)11-

InchiKey: MMTYCZHALNNXSN-UHFFFAOYSA-N

Formula: C18H25ClO4

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

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-283.63	kJ/mol	Joback Method
hf	-710.97	kJ/mol	Joback Method
hfus	35.23	kJ/mol	Joback Method
hvap	80.13	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.639		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	2268.00		NIST Webbook
rinpol	2268.00		NIST Webbook
tb	831.59	K	Joback Method
tc	1042.66	K	Joback Method
tf	460.80	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.03	J/mol×K	831.59	Joback Method
cpg	805.01	J/mol×K	866.77	Joback Method
cpg	818.82	J/mol×K	901.95	Joback Method
cpg	831.48	J/mol×K	937.12	Joback Method
cpg	843.02	J/mol×K	972.30	Joback Method
cpg	853.45	J/mol×K	1007.48	Joback Method
cpg	862.79	J/mol×K	1042.66	Joback Method
dvisc	0.0008911	Pa×s	460.80	Joback Method

dvisc	0.0004117	Pa×s	522.60	Joback Method
dvisc	0.0002240	Pa×s	584.40	Joback Method
dvisc	0.0001369	Pa×s	646.19	Joback Method
dvisc	0.0000912	Pa×s	707.99	Joback Method
dvisc	0.0000648	Pa×s	769.79	Joback Method
dvisc	0.0000485	Pa×s	831.59	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=U393481&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