Glutaric acid, 3-chlorophenyl 3-phenylpropyl ester

Inchi: InChI=1S/C20H21ClO4/c21-17-10-4-11-18(15-17)25-20(23)13-5-12-19(22)24-14-6-9-16-

InchiKey: BEHDRXANRCVTKN-UHFFFAOYSA-N

Formula: C20H21ClO4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)OCCCc1ccccc1

Mol. weight [g/mol]: 360.83

Physical Properties

Property code	Value	Unit	Source
gf	-147.06	kJ/mol	Joback Method
hf	-499.88	kJ/mol	Joback Method
hfus	45.02	kJ/mol	Joback Method
hvap	88.02	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.592		Crippen Method
mcvol	272.260	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	2817.00		NIST Webbook
rinpol	2817.00		NIST Webbook
tb	905.35	K	Joback Method
tc	1132.67	K	Joback Method
tf	554.76	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.72	J/mol×K	905.35	Joback Method
cpg	817.53	J/mol×K	943.24	Joback Method
cpg	829.07	J/mol×K	981.12	Joback Method
cpg	839.40	J/mol×K	1019.01	Joback Method
cpg	848.54	J/mol×K	1056.90	Joback Method
cpg	856.55	J/mol×K	1094.79	Joback Method
cpg	863.47	J/mol×K	1132.67	Joback Method
dvisc	0.0004278	Pa×s	554.76	Joback Method

dvisc	0.0002505	Pa×s	613.19	Joback Method
dvisc	0.0001609	Pa×s	671.62	Joback Method
dvisc	0.0001110	Pa×s	730.05	Joback Method
dvisc	0.0000809	Pa×s	788.49	Joback Method
dvisc	0.0000616	Pa×s	846.92	Joback Method
dvisc	0.0000486	Pa×s	905.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391779&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

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