Glutaric acid, 3-chlorophenyl 2,6-dichlorophenyl ester

Inchi: InChI=1S/C17H13Cl3O4/c18-11-4-1-5-12(10-11)23-15(21)8-3-9-16(22)24-17-13(19)6-2-7

InchiKey: SUGKFGTXVTVASX-UHFFFAOYSA-N

Formula: C17H13Cl3O4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cccc1Cl)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 387.64

Physical Properties

Property code	Value	Unit	Source
gf	-215.44	kJ/mol	Joback Method
hf	-492.38	kJ/mol	Joback Method
hfus	44.87	kJ/mol	Joback Method
hvap	91.44	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.328		Crippen Method
mcvol	254.470	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2828.00		NIST Webbook
rinpol	2828.00		NIST Webbook
tb	921.53	K	Joback Method
tc	1162.77	K	Joback Method
tf	605.83	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.67	J/mol×K	921.53	Joback Method
cpg	682.15	J/mol×K	961.74	Joback Method
cpg	690.43	J/mol×K	1001.94	Joback Method
cpg	697.53	J/mol×K	1042.15	Joback Method
cpg	703.48	J/mol×K	1082.35	Joback Method
cpg	708.30	J/mol×K	1122.56	Joback Method
cpg	712.03	J/mol×K	1162.77	Joback Method
dvisc	0.0003250	Pa×s	605.83	Joback Method

dvisc	0.0002167	Pa×s	658.45	Joback Method
dvisc	0.0001534	Pa×s	711.06	Joback Method
dvisc	0.0001138	Pa×s	763.68	Joback Method
dvisc	0.0000878	Pa×s	816.30	Joback Method
dvisc	0.0000699	Pa×s	868.91	Joback Method
dvisc	0.0000571	Pa×s	921.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390262&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