Glutaric acid, 3-chlorophenyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C17H12Cl4O4/c18-10-3-1-4-11(7-10)24-16(22)5-2-6-17(23)25-15-9-13(20)12(
InchiKey: NLUWQWUSHBZSDM-UHFFFAOYSA-N
Formula: C17H12Cl4O4
SMILES: O=C(CCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 422.09

Physical Properties

Property code	Value	Unit	Source
gf	-237.00	kJ/mol	Joback Method
hf	-519.59	kJ/mol	Joback Method
hfus	48.67	kJ/mol	Joback Method
hvap	96.49	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	5.981		Crippen Method
mcvol	266.710	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	3015.00		NIST Webbook
rinpol	3015.00		NIST Webbook
tb	963.94	K	Joback Method
tc	1208.81	K	Joback Method
tf	648.27	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.12	J/mol×K	963.94	Joback Method
cpg	696.16	J/mol×K	1004.75	Joback Method
cpg	702.98	J/mol×K	1045.56	Joback Method
cpg	708.60	J/mol×K	1086.37	Joback Method
cpg	713.06	J/mol×K	1127.19	Joback Method
cpg	716.37	J/mol×K	1168.00	Joback Method
cpg	718.54	J/mol×K	1208.81	Joback Method
dvisc	0.0002501	Pa×s	648.27	Joback Method

dvisc	0.0001728	Pa×s	700.88	Joback Method
dvisc	0.0001257	Pa×s	753.49	Joback Method
dvisc	0.0000953	Pa×s	806.11	Joback Method
dvisc	0.0000748	Pa×s	858.72	Joback Method
dvisc	0.0000603	Pa×s	911.33	Joback Method
dvisc	0.0000498	Pa×s	963.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392167&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