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

Inchi: InChI=1S/C17H11Cl5O4/c18-9-3-1-4-13(17(9)22)25-15(23)5-2-6-16(24)26-14-8-11(20)10

InchiKey: IGSBBTZEVWLIOR-UHFFFAOYSA-N

Formula: C17H11Cl5O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 456.53

Physical Properties

Property code	Value	Unit	Source
gf	-258.56	kJ/mol	Joback Method
hf	-546.80	kJ/mol	Joback Method
hfus	52.48	kJ/mol	Joback Method
hvap	101.53	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	6.635		Crippen Method
mcvol	278.950	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	3235.00		NIST Webbook
rinpol	3235.00		NIST Webbook
tb	1006.35	K	Joback Method
tc	1255.15	K	Joback Method
tf	690.71	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.63	J/mol×K	1006.35	Joback Method
cpg	722.23	J/mol×K	1213.68	Joback Method
cpg	720.53	J/mol×K	1172.22	Joback Method
cpg	717.64	J/mol×K	1130.75	Joback Method
cpg	713.54	J/mol×K	1089.28	Joback Method
cpg	708.20	J/mol×K	1047.82	Joback Method
cpg	722.75	J/mol×K	1255.15	Joback Method
dvisc	0.0000432	Pa×s	1006.35	Joback Method

dvisc	0.0000518	Pa×s	953.74	Joback Method
dvisc	0.0000635	Pa×s	901.14	Joback Method
dvisc	0.0000797	Pa×s	848.53	Joback Method
dvisc	0.0001032	Pa×s	795.92	Joback Method
dvisc	0.0001386	Pa×s	743.32	Joback Method
dvisc	0.0001947	Pa×s	690.71	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=U392169&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