Glutaric acid, 2,4,6-trichlorophenyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C17H10Cl6O4/c18-8-4-12(22)17(13(23)5-8)27-16(25)3-1-2-15(24)26-14-7-10(

InchiKey: WJOUHFPSLYRCFG-UHFFFAOYSA-N

Formula: C17H10Cl6O4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 490.98

Physical Properties

Property code	Value	Unit	Source
gf	-280.12	kJ/mol	Joback Method
hf	-574.01	kJ/mol	Joback Method
hfus	56.29	kJ/mol	Joback Method
hvap	106.58	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.288		Crippen Method
mcvol	291.190	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	1048.76	K	Joback Method
tc	1301.89	K	Joback Method
tf	733.15	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.22	J/mol×K	1048.76	Joback Method
cpg	718.29	J/mol×K	1090.95	Joback Method
cpg	722.07	J/mol×K	1133.14	Joback Method
cpg	724.57	J/mol×K	1175.32	Joback Method
cpg	725.80	J/mol×K	1217.51	Joback Method
cpg	725.76	J/mol×K	1259.70	Joback Method
cpg	724.48	J/mol×K	1301.89	Joback Method
dvisc	0.0001529	Pa×s	733.15	Joback Method

dvisc	0.0001118	Pa×s	785.75	Joback Method
dvisc	0.0000850	Pa×s	838.35	Joback Method
dvisc	0.0000667	Pa×s	890.96	Joback Method
dvisc	0.0000538	Pa×s	943.56	Joback Method
dvisc	0.0000444	Pa×s	996.16	Joback Method
dvisc	0.0000373	Pa×s	1048.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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