Glutaric acid, 2,4,6-trichlorophenyl 2-methyl-4-chlorophenyl ester

Inchi: InChI=1S/C18H14Cl4O4/c1-10-7-11(19)5-6-15(10)25-16(23)3-2-4-17(24)26-18-13(21)8-1

InchiKey: DOXSHFIRRCDLQW-UHFFFAOYSA-N

Formula: C18H14Cl4O4

SMILES: Cc1cc(Cl)ccc1OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 436.11

Physical Properties

Property code	Value	Unit	Source
gf	-238.21	kJ/mol	Joback Method
hf	-551.70	kJ/mol	Joback Method
hfus	50.88	kJ/mol	Joback Method
hvap	99.38	kJ/mol	Joback Method
log10ws	-7.38		Crippen Method
logp	6.290		Crippen Method
mcvol	280.800	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	3087.00		NIST Webbook
rinpol	3087.00		NIST Webbook
tb	991.80	K	Joback Method
tc	1235.66	K	Joback Method
tf	672.06	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.11	J/mol×K	991.80	Joback Method
cpg	769.63	J/mol×K	1195.02	Joback Method
cpg	766.63	J/mol×K	1154.38	Joback Method
cpg	762.39	J/mol×K	1113.73	Joback Method
cpg	756.90	J/mol×K	1073.09	Joback Method
cpg	750.14	J/mol×K	1032.44	Joback Method
cpg	771.42	J/mol×K	1235.66	Joback Method
dvisc	0.0000441	Pa×s	991.80	Joback Method

dvisc	0.0000531	Pa×s	938.51	Joback Method
dvisc	0.0000653	Pa×s	885.22	Joback Method
dvisc	0.0000825	Pa×s	831.93	Joback Method
dvisc	0.0001077	Pa×s	778.64	Joback Method
dvisc	0.0001462	Pa×s	725.35	Joback Method
dvisc	0.0002083	Pa×s	672.06	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392079&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

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