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

Inchi: InChI=1S/C16H17Cl3O4/c17-10-8-12(18)16(13(19)9-10)23-15(21)7-3-6-14(20)22-11-4-1

InchiKey: YFJYWQFLHUQBRA-UHFFFAOYSA-N

Formula: C16H17Cl3O4

SMILES: O=C(CCCC(=O)OC1CCCC1)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 379.66

Physical Properties

Property code	Value	Unit	Source
gf	-299.72	kJ/mol	Joback Method
hf	-647.79	kJ/mol	Joback Method
hfus	42.17	kJ/mol	Joback Method
hvap	87.20	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.208		Crippen Method
mcvol	253.280	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
tb	887.25	K	Joback Method
tc	1120.89	K	Joback Method
tf	579.04	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.08	J/mol×K	887.25	Joback Method
cpg	721.04	J/mol×K	926.19	Joback Method
cpg	731.75	J/mol×K	965.13	Joback Method
cpg	741.22	J/mol×K	1004.07	Joback Method
cpg	749.48	J/mol×K	1043.01	Joback Method
cpg	756.55	J/mol×K	1081.95	Joback Method
cpg	762.47	J/mol×K	1120.89	Joback Method
dvisc	0.0005341	Pa×s	579.04	Joback Method

dvisc	0.0003573	Pa×s	630.41	Joback Method
dvisc	0.0002539	Pa×s	681.78	Joback Method
dvisc	0.0001893	Pa×s	733.14	Joback Method
dvisc	0.0001466	Pa×s	784.51	Joback Method
dvisc	0.0001172	Pa×s	835.88	Joback Method
dvisc	0.0000962	Pa×s	887.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405401&Units=SI

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