Glutaric acid, hexa-1,5-dien-3-yl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C17H17Cl3O4/c1-3-6-12(4-2)23-15(21)7-5-8-16(22)24-17-13(19)9-11(18)10-14

InchiKey: KTMCAEBJFPYSCZ-UHFFFAOYSA-N

Formula: C17H17Cl3O4

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

Mol. weight [g/mol]: 391.67

Physical Properties

Property code	Value	Unit	Source
gf	-154.61	kJ/mol	Joback Method
hf	-483.33	kJ/mol	Joback Method
hfus	44.74	kJ/mol	Joback Method
hvap	87.44	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	5.396		Crippen Method
mcvol	269.630	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2462.00		NIST Webbook
rinpol	2462.00		NIST Webbook
tb	887.77	K	Joback Method
tc	1108.91	K	Joback Method
tf	560.89	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.91	J/mol×K	887.77	Joback Method
cpg	732.85	J/mol×K	924.63	Joback Method
cpg	742.78	J/mol×K	961.48	Joback Method
cpg	751.71	J/mol×K	998.34	Joback Method
cpg	759.69	J/mol×K	1035.20	Joback Method
cpg	766.71	J/mol×K	1072.06	Joback Method
cpg	772.82	J/mol×K	1108.91	Joback Method
dvisc	0.0004036	Pa×s	560.89	Joback Method

dvisc	0.0002534	Pa×s	615.37	Joback Method
dvisc	0.0001716	Pa×s	669.85	Joback Method
dvisc	0.0001232	Pa×s	724.33	Joback Method
dvisc	0.0000927	Pa×s	778.81	Joback Method
dvisc	0.0000724	Pa×s	833.29	Joback Method
dvisc	0.0000582	Pa×s	887.77	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=U405288&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