Glutaric acid, 2-methylpent-3-yl 2,6-dichlorophenyl ester

Inchi: InChI=1S/C17H22Cl2O4/c1-4-14(11(2)3)22-15(20)9-6-10-16(21)23-17-12(18)7-5-8-13(1
InchiKey: IFQVQAYLHCMKER-UHFFFAOYSA-N
Formula: C17H22Cl2O4
SMILES: CCC(OC(=O)CCCC(=O)Oc1c(Cl)cccc1Cl)C(C)C
Mol. weight [g/mol]: 361.26

Physical Properties

Property code	Value	Unit	Source
gf	-311.17	kJ/mol	Joback Method
hf	-712.26	kJ/mol	Joback Method
hfus	39.97	kJ/mol	Joback Method
hvap	83.34	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.047		Crippen Method
mcvol	265.990	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tb	851.56	K	Joback Method
tc	1065.87	K	Joback Method
tf	506.97	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.37	J/mol×K	851.56	Joback Method
cpg	811.90	J/mol×K	1030.16	Joback Method
cpg	802.96	J/mol×K	994.44	Joback Method
cpg	792.96	J/mol×K	958.72	Joback Method
cpg	781.87	J/mol×K	923.00	Joback Method
cpg	769.68	J/mol×K	887.28	Joback Method
cpg	819.79	J/mol×K	1065.87	Joback Method
dvisc	0.0000532	Pa×s	851.56	Joback Method

dvisc	0.0000686	Pa×s	794.13	Joback Method
dvisc	0.0000920	Pa×s	736.70	Joback Method
dvisc	0.0001298	Pa×s	679.26	Joback Method
dvisc	0.0001951	Pa×s	621.83	Joback Method
dvisc	0.0003186	Pa×s	564.40	Joback Method
dvisc	0.0005814	Pa×s	506.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390253&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