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

Inchi: InChI=1S/C20H19Cl3O5/c1-12(2)26-16-6-3-4-7-17(16)27-18(24)8-5-9-19(25)28-20-14(22
InchiKey: UEABWCZPIMGXFL-UHFFFAOYSA-N
Formula: C20H19Cl3O5
SMILES: CC(C)Oc1ccccc1OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 445.72

Physical Properties

Property code	Value	Unit	Source
gf	-307.25	kJ/mol	Joback Method
hf	-703.27	kJ/mol	Joback Method
hfus	49.91	kJ/mol	Joback Method
hvap	100.80	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	6.115		Crippen Method
mcvol	302.610	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	3029.00		NIST Webbook
rinpol	3029.00		NIST Webbook
tb	1017.13	K	Joback Method
tc	1257.25	K	Joback Method
tf	659.39	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.97	J/mol×K	1017.13	Joback Method
cpg	873.56	J/mol×K	1057.15	Joback Method
cpg	880.60	J/mol×K	1097.17	Joback Method
cpg	886.11	J/mol×K	1137.19	Joback Method
cpg	890.09	J/mol×K	1177.21	Joback Method
cpg	892.55	J/mol×K	1217.23	Joback Method
cpg	893.50	J/mol×K	1257.25	Joback Method
dvisc	0.0001610	Pa×s	659.39	Joback Method

dvisc	0.0001041	Pa×s	719.01	Joback Method
dvisc	0.0000720	Pa×s	778.64	Joback Method
dvisc	0.0000524	Pa×s	838.26	Joback Method
dvisc	0.0000399	Pa×s	897.88	Joback Method
dvisc	0.0000313	Pa×s	957.51	Joback Method
dvisc	0.0000253	Pa×s	1017.13	Joback Method

Sources

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=U391877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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