Glutaric acid, dodec-2-en-1-yl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C23H31Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-15-29-21(27)13-12-14-22(28)30-20-17

InchiKey: DTMMDEHJTZDINC-ZHACJKMWSA-N

Formula: C23H31Cl3O4

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl

Mol. weight [g/mol]: 477.85

Physical Properties

Property code	Value	Unit	Source
gf	-197.11	kJ/mol	Joback Method
hf	-735.53	kJ/mol	Joback Method
hfus	66.57	kJ/mol	Joback Method
hvap	102.48	kJ/mol	Joback Method
log10ws	-8.84		Crippen Method
logp	7.963		Crippen Method
mcvol	358.470	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	3251.00		NIST Webbook
rinpol	3251.00		NIST Webbook
tb	1036.29	K	Joback Method
tc	1268.71	K	Joback Method
tf	641.95	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1100.85	J/mol×K	1036.29	Joback Method
cpg	1113.76	J/mol×K	1075.03	Joback Method
cpg	1125.39	J/mol×K	1113.76	Joback Method
cpg	1135.80	J/mol×K	1152.50	Joback Method
cpg	1145.03	J/mol×K	1191.24	Joback Method
cpg	1153.15	J/mol×K	1229.97	Joback Method
cpg	1160.22	J/mol×K	1268.71	Joback Method
dvisc	0.0001644	Pa×s	641.95	Joback Method

dvisc	0.0000979	Pa×s	707.67	Joback Method
dvisc	0.0000637	Pa×s	773.40	Joback Method
dvisc	0.0000443	Pa×s	839.12	Joback Method
dvisc	0.0000325	Pa×s	904.84	Joback Method
dvisc	0.0000249	Pa×s	970.57	Joback Method
dvisc	0.0000197	Pa×s	1036.29	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=U392190&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