Glutaric acid, 2,4,6-trichlorophenyl 10-chlorodecyl ester

Inchi: InChI=1S/C21H28Cl4O4/c22-12-7-5-3-1-2-4-6-8-13-28-19(26)10-9-11-20(27)29-21-17(24
InchiKey: XORGHWNRWGQJLU-UHFFFAOYSA-N
Formula: C21H28Cl4O4
SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCCCCCCCCCCCCl
Mol. weight [g/mol]: 486.26

Physical Properties

Property code	Value	Unit	Source
gf	-306.10	kJ/mol	Joback Method
hf	-827.21	kJ/mol	Joback Method
hfus	65.38	kJ/mol	Joback Method
hvap	102.45	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.625		Crippen Method
mcvol	346.830	ml/mol	McGowan Method
pc	1108.15	kPa	Joback Method
rinpol	3349.00		NIST Webbook
rinpol	3349.00		NIST Webbook
tb	1023.80	K	Joback Method
tc	1253.62	K	Joback Method
tf	654.41	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.99	J/mol×K	1023.80	Joback Method
cpg	1042.38	J/mol×K	1062.10	Joback Method
cpg	1052.43	J/mol×K	1100.41	Joback Method
cpg	1061.16	J/mol×K	1138.71	Joback Method
cpg	1068.61	J/mol×K	1177.02	Joback Method
cpg	1074.81	J/mol×K	1215.32	Joback Method
cpg	1079.80	J/mol×K	1253.62	Joback Method
dvisc	0.0001838	Pa×s	654.41	Joback Method

dvisc	0.0001147	Pa×s	715.98	Joback Method
dvisc	0.0000771	Pa×s	777.54	Joback Method
dvisc	0.0000550	Pa×s	839.11	Joback Method
dvisc	0.0000410	Pa×s	900.67	Joback Method
dvisc	0.0000318	Pa×s	962.23	Joback Method
dvisc	0.0000254	Pa×s	1023.80	Joback Method

Sources

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=U392477&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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