Glutaric acid, 3-chlorophenyl 10-chlorodecyl ester

Inchi: InChI=1S/C21H30Cl2O4/c22-15-7-5-3-1-2-4-6-8-16-26-20(24)13-10-14-21(25)27-19-12-9

InchiKey: SOBHDGZJBVRIMH-UHFFFAOYSA-N

Formula: C21H30Cl2O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)OCCCCCCCCCCCCl

Mol. weight [g/mol]: 417.37

Physical Properties

Property code	Value	Unit	Source
gf	-262.98	kJ/mol	Joback Method
hf	-772.79	kJ/mol	Joback Method
hfus	57.77	kJ/mol	Joback Method
hvap	92.36	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.318		Crippen Method
mcvol	322.350	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
rinpol	3085.00		NIST Webbook
rinpol	3085.00		NIST Webbook
tb	938.98	K	Joback Method
tc	1152.41	K	Joback Method
tf	569.53	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.47	J/mol×K	938.98	Joback Method
cpg	1003.48	J/mol×K	974.55	Joback Method
cpg	1016.27	J/mol×K	1010.12	Joback Method
cpg	1027.86	J/mol×K	1045.69	Joback Method
cpg	1038.30	J/mol×K	1081.26	Joback Method
cpg	1047.61	J/mol×K	1116.84	Joback Method
cpg	1055.84	J/mol×K	1152.41	Joback Method
dvisc	0.0003497	Pa×s	569.53	Joback Method

dvisc	0.0001970	Pa×s	631.11	Joback Method
dvisc	0.0001229	Pa×s	692.68	Joback Method
dvisc	0.0000828	Pa×s	754.25	Joback Method
dvisc	0.0000592	Pa×s	815.83	Joback Method
dvisc	0.0000444	Pa×s	877.40	Joback Method
dvisc	0.0000346	Pa×s	938.98	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=U392470&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