Glutaric acid, 2,3-dichlorophenyl 10-chlorodecyl ester

Inchi: InChI=1S/C21H29Cl3O4/c22-15-7-5-3-1-2-4-6-8-16-27-19(25)13-10-14-20(26)28-18-12-9

InchiKey: MGGDMXNYLPMZOC-UHFFFAOYSA-N

Formula: C21H29Cl3O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)OCCCCCCCCCCCCl

Mol. weight [g/mol]: 451.81

Physical Properties

Property code	Value	Unit	Source
gf	-284.54	kJ/mol	Joback Method
hf	-800.00	kJ/mol	Joback Method
hfus	61.57	kJ/mol	Joback Method
hvap	97.41	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	6.972		Crippen Method
mcvol	334.590	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	3297.00		NIST Webbook
rinpol	3297.00		NIST Webbook
tb	981.39	K	Joback Method
tc	1202.67	K	Joback Method
tf	611.97	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.40	J/mol×K	981.39	Joback Method
cpg	1024.13	J/mol×K	1018.27	Joback Method
cpg	1035.58	J/mol×K	1055.15	Joback Method
cpg	1045.79	J/mol×K	1092.03	Joback Method
cpg	1054.79	J/mol×K	1128.91	Joback Method
cpg	1062.61	J/mol×K	1165.79	Joback Method
cpg	1069.29	J/mol×K	1202.67	Joback Method
dvisc	0.0002508	Pa×s	611.97	Joback Method

dvisc	0.0001494	Pa×s	673.54	Joback Method
dvisc	0.0000970	Pa×s	735.11	Joback Method
dvisc	0.0000674	Pa×s	796.68	Joback Method
dvisc	0.0000493	Pa×s	858.25	Joback Method
dvisc	0.0000376	Pa×s	919.82	Joback Method
dvisc	0.0000297	Pa×s	981.39	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=U392475&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