Glutaric acid, 2,4,6-trichlorophenyl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C21H29Cl3O4/c1-14(2)6-4-7-15(3)10-11-27-19(25)8-5-9-20(26)28-21-17(23)12
InchiKey: SVAJLRFUOHVUBF-UHFFFAOYSA-N
Formula: C21H29Cl3O4
SMILES: CC(C)CCCC(C)CCOC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 451.81

Physical Properties

Property code	Value	Unit	Source
gf	-299.05	kJ/mol	Joback Method
hf	-822.03	kJ/mol	Joback Method
hfus	54.14	kJ/mol	Joback Method
hvap	97.29	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.118		Crippen Method
mcvol	334.590	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2917.00		NIST Webbook
rinpol	2917.00		NIST Webbook
tb	985.49	K	Joback Method
tc	1209.07	K	Joback Method
tf	594.49	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.97	J/mol×K	985.49	Joback Method
cpg	1060.48	J/mol×K	1171.80	Joback Method
cpg	1053.17	J/mol×K	1134.54	Joback Method
cpg	1044.60	J/mol×K	1097.28	Joback Method
cpg	1034.72	J/mol×K	1060.02	Joback Method
cpg	1023.52	J/mol×K	1022.75	Joback Method
cpg	1066.54	J/mol×K	1209.07	Joback Method
dvisc	0.0000252	Pa×s	985.49	Joback Method

dvisc	0.0000324	Pa×s	920.32	Joback Method
dvisc	0.0000433	Pa×s	855.16	Joback Method
dvisc	0.0000606	Pa×s	789.99	Joback Method
dvisc	0.0000902	Pa×s	724.82	Joback Method
dvisc	0.0001452	Pa×s	659.66	Joback Method
dvisc	0.0002594	Pa×s	594.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391492&Units=SI
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

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