Glutaric acid, 2,4,6-trichlorophenyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H23Cl3O4/c1-4-6-15(11(2)3)24-16(22)7-5-8-17(23)25-18-13(20)9-12(19)10

InchiKey: LKJWLZSZBZQUBO-UHFFFAOYSA-N

Formula: C18H23Cl3O4

SMILES: CCCC(OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)C(C)C

Mol. weight [g/mol]: 409.73

Physical Properties

Property code	Value	Unit	Source
gf	-324.31	kJ/mol	Joback Method
hf	-760.11	kJ/mol	Joback Method
hfus	46.37	kJ/mol	Joback Method
hvap	90.61	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.090		Crippen Method
mcvol	292.320	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	2540.00		NIST Webbook
rinpol	2540.00		NIST Webbook
tb	916.85	K	Joback Method
tc	1135.89	K	Joback Method
tf	560.68	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.30	J/mol×K	916.85	Joback Method
cpg	847.45	J/mol×K	953.36	Joback Method
cpg	858.41	J/mol×K	989.86	Joback Method
cpg	868.20	J/mol×K	1026.37	Joback Method
cpg	876.84	J/mol×K	1062.88	Joback Method
cpg	884.33	J/mol×K	1099.38	Joback Method
cpg	890.71	J/mol×K	1135.89	Joback Method
dvisc	0.0003680	Pa×s	560.68	Joback Method

dvisc	0.0002127	Pa×s	620.04	Joback Method
dvisc	0.0001353	Pa×s	679.40	Joback Method
dvisc	0.0000925	Pa×s	738.77	Joback Method
dvisc	0.0000670	Pa×s	798.13	Joback Method
dvisc	0.0000507	Pa×s	857.49	Joback Method
dvisc	0.0000398	Pa×s	916.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393844&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