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

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

InchiKey: SKAWSJJGEANSOY-UHFFFAOYSA-N

Formula: C18H23Cl3O4

SMILES: CC(C)C(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	-326.75	kJ/mol	Joback Method
hf	-765.39	kJ/mol	Joback Method
hfus	42.85	kJ/mol	Joback Method
hvap	90.23	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.946		Crippen Method
mcvol	292.320	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	2539.00		NIST Webbook
rinpol	2539.00		NIST Webbook
tb	916.41	K	Joback Method
tc	1137.44	K	Joback Method
tf	545.68	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.82	J/mol×K	916.41	Joback Method
cpg	848.04	J/mol×K	953.25	Joback Method
cpg	859.03	J/mol×K	990.09	Joback Method
cpg	868.82	J/mol×K	1026.93	Joback Method
cpg	877.42	J/mol×K	1063.76	Joback Method
cpg	884.85	J/mol×K	1100.60	Joback Method
cpg	891.13	J/mol×K	1137.44	Joback Method
dvisc	0.0004038	Pa×s	545.68	Joback Method

dvisc	0.0002204	Pa×s	607.47	Joback Method
dvisc	0.0001345	Pa×s	669.26	Joback Method
dvisc	0.0000892	Pa×s	731.05	Joback Method
dvisc	0.0000631	Pa×s	792.83	Joback Method
dvisc	0.0000469	Pa×s	854.62	Joback Method
dvisc	0.0000363	Pa×s	916.41	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=U393485&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