Glutaric acid, 2,4,6-trichlorophenyl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C18H23Cl3O5/c1-12(6-8-24-2)7-9-25-16(22)4-3-5-17(23)26-18-14(20)10-13(19

InchiKey: SJVCCNBBUMXNCX-UHFFFAOYSA-N

Formula: C18H23Cl3O5

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

Mol. weight [g/mol]: 425.73

Physical Properties

Property code	Value	Unit	Source
gf	-426.87	kJ/mol	Joback Method
hf	-887.05	kJ/mol	Joback Method
hfus	51.08	kJ/mol	Joback Method
hvap	93.41	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.328		Crippen Method
mcvol	298.190	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2769.00		NIST Webbook
rinpol	2769.00		NIST Webbook
tb	939.71	K	Joback Method
tc	1158.25	K	Joback Method
tf	597.91	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.06	J/mol×K	939.71	Joback Method
cpg	872.45	J/mol×K	976.13	Joback Method
cpg	882.54	J/mol×K	1012.56	Joback Method
cpg	891.35	J/mol×K	1048.98	Joback Method
cpg	898.86	J/mol×K	1085.41	Joback Method
cpg	905.08	J/mol×K	1121.83	Joback Method
cpg	910.01	J/mol×K	1158.25	Joback Method
dvisc	0.0002396	Pa×s	597.91	Joback Method

dvisc	0.0001483	Pa×s	654.88	Joback Method
dvisc	0.0000992	Pa×s	711.84	Joback Method
dvisc	0.0000704	Pa×s	768.81	Joback Method
dvisc	0.0000524	Pa×s	825.78	Joback Method
dvisc	0.0000405	Pa×s	882.74	Joback Method
dvisc	0.0000323	Pa×s	939.71	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=U393531&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