Fumaric acid, ethyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C12H9Cl3O4/c1-2-18-10(16)3-4-11(17)19-12-8(14)5-7(13)6-9(12)15/h3-6H,2H
InchiKey: ZQUKPRSELNYMAD-ONEGZZNKSA-N
Formula: C12H9Cl3O4
SMILES: CCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 323.56

Physical Properties

Property code	Value	Unit	Source
gf	-289.73	kJ/mol	Joback Method
hf	-508.49	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	77.99	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.671		Crippen Method
mcvol	203.480	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	2059.00		NIST Webbook
rinpol	2059.00		NIST Webbook
tb	784.61	K	Joback Method
tc	1014.85	K	Joback Method
tf	517.98	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.14	J/mol×K	784.61	Joback Method
cpg	486.61	J/mol×K	822.98	Joback Method
cpg	495.27	J/mol×K	861.36	Joback Method
cpg	503.14	J/mol×K	899.73	Joback Method
cpg	510.23	J/mol×K	938.11	Joback Method
cpg	516.55	J/mol×K	976.48	Joback Method
cpg	522.10	J/mol×K	1014.85	Joback Method
dvisc	0.0005116	Pa×s	517.98	Joback Method

dvisc	0.0003469	Pa×s	562.42	Joback Method
dvisc	0.0002490	Pa×s	606.86	Joback Method
dvisc	0.0001870	Pa×s	651.30	Joback Method
dvisc	0.0001457	Pa×s	695.73	Joback Method
dvisc	0.0001169	Pa×s	740.17	Joback Method
dvisc	0.0000962	Pa×s	784.61	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348267&Units=SI

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