Fumaric acid, ethyl 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C12H8Cl4O4/c1-2-19-8(17)3-4-9(18)20-12-7(14)5-6(13)10(15)11(12)16/h3-5H
InchiKey: VOYOQIXZKUBDBK-ONEGZZNKSA-N
Formula: C12H8Cl4O4
SMILES: CCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 358.00

Physical Properties

Property code	Value	Unit	Source
gf	-311.29	kJ/mol	Joback Method
hf	-535.70	kJ/mol	Joback Method
hfus	41.88	kJ/mol	Joback Method
hvap	83.04	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.325		Crippen Method
mcvol	215.720	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	2274.00		NIST Webbook
rinpol	2274.00		NIST Webbook
tb	827.02	K	Joback Method
tc	1060.57	K	Joback Method
tf	560.42	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.07	J/mol×K	827.02	Joback Method
cpg	528.08	J/mol×K	1021.64	Joback Method
cpg	522.86	J/mol×K	982.72	Joback Method
cpg	516.85	J/mol×K	943.79	Joback Method
cpg	510.05	J/mol×K	904.87	Joback Method
cpg	502.46	J/mol×K	865.94	Joback Method
cpg	532.52	J/mol×K	1060.57	Joback Method
dvisc	0.0000853	Pa×s	827.02	Joback Method

dvisc	0.0001025	Pa×s	782.59	Joback Method
dvisc	0.0001258	Pa×s	738.15	Joback Method
dvisc	0.0001586	Pa×s	693.72	Joback Method
dvisc	0.0002063	Pa×s	649.29	Joback Method
dvisc	0.0002790	Pa×s	604.85	Joback Method
dvisc	0.0003957	Pa×s	560.42	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=U348192&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