Fumaric acid, ethyl pentachlorophenyl ester

Inchi: InChI=1S/C12H7Cl5O4/c1-2-20-5(18)3-4-6(19)21-12-10(16)8(14)7(13)9(15)11(12)17/h3-
InchiKey: MSJGEMUIWSXWBP-ONEGZZNKSA-N
Formula: C12H7Cl5O4
SMILES: CCOC(=O)C=CC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 392.45

Physical Properties

Property code	Value	Unit	Source
gf	-332.85	kJ/mol	Joback Method
hf	-562.91	kJ/mol	Joback Method
hfus	45.69	kJ/mol	Joback Method
hvap	88.09	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.978		Crippen Method
mcvol	227.960	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	2474.00		NIST Webbook
rinpol	2474.00		NIST Webbook
tb	869.43	K	Joback Method
tc	1106.28	K	Joback Method
tf	602.86	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.35	J/mol×K	869.43	Joback Method
cpg	516.67	J/mol×K	908.91	Joback Method
cpg	523.19	J/mol×K	948.38	Joback Method
cpg	528.91	J/mol×K	987.86	Joback Method
cpg	533.81	J/mol×K	1027.33	Joback Method
cpg	537.91	J/mol×K	1066.81	Joback Method
cpg	541.19	J/mol×K	1106.28	Joback Method
dvisc	0.0003100	Pa×s	602.86	Joback Method

dvisc	0.0002257	Pa×s	647.29	Joback Method
dvisc	0.0001712	Pa×s	691.72	Joback Method
dvisc	0.0001342	Pa×s	736.14	Joback Method
dvisc	0.0001082	Pa×s	780.57	Joback Method
dvisc	0.0000893	Pa×s	825.00	Joback Method
dvisc	0.0000751	Pa×s	869.43	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=U348178&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