Fumaric acid, pentachlorophenyl propyl ester

Inchi: InChI=1S/C13H9Cl5O4/c1-2-5-21-6(19)3-4-7(20)22-13-11(17)9(15)8(14)10(16)12(13)18/
InchiKey: SZMBLVSWIKXQFX-ONEGZZNKSA-N
Formula: C13H9Cl5O4
SMILES: CCCOC(=O)C=CC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 406.47

Physical Properties

Property code	Value	Unit	Source
gf	-324.43	kJ/mol	Joback Method
hf	-583.55	kJ/mol	Joback Method
hfus	48.28	kJ/mol	Joback Method
hvap	90.31	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.368		Crippen Method
mcvol	242.050	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	2589.00		NIST Webbook
tb	892.31	K	Joback Method
tc	1126.39	K	Joback Method
tf	614.13	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.69	J/mol×K	892.31	Joback Method
cpg	570.47	J/mol×K	931.32	Joback Method
cpg	577.39	J/mol×K	970.34	Joback Method
cpg	583.47	J/mol×K	1009.35	Joback Method
cpg	588.70	J/mol×K	1048.36	Joback Method
cpg	593.09	J/mol×K	1087.37	Joback Method
cpg	596.64	J/mol×K	1126.39	Joback Method
dvisc	0.0002818	Pa×s	614.13	Joback Method
dvisc	0.0002028	Pa×s	660.49	Joback Method

dvisc	0.0001523	Pa×s	706.86	Joback Method
dvisc	0.0001185	Pa×s	753.22	Joback Method
dvisc	0.0000949	Pa×s	799.58	Joback Method
dvisc	0.0000779	Pa×s	845.95	Joback Method
dvisc	0.0000653	Pa×s	892.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348179&Units=SI
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

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