Fumaric acid, propyl 2,3,4,5-tetrachlorophenyl ester

Inchi: InChI=1S/C13H10Cl4O4/c1-2-5-20-9(18)3-4-10(19)21-8-6-7(14)11(15)13(17)12(8)16/h3-

InchiKey: AEDTXMHHILJJGC-ONEGZZNKSA-N

Formula: C13H10Cl4O4

SMILES: CCCOC(=O)C=CC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 372.03

Physical Properties

Property code	Value	Unit	Source
gf	-302.87	kJ/mol	Joback Method
hf	-556.34	kJ/mol	Joback Method
hfus	44.47	kJ/mol	Joback Method
hvap	85.27	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.715		Crippen Method
mcvol	229.810	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	2460.00		NIST Webbook
tb	849.90	K	Joback Method
tc	1080.33	K	Joback Method
tf	571.69	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.94	J/mol×K	849.90	Joback Method
cpg	582.97	J/mol×K	1041.93	Joback Method
cpg	577.41	J/mol×K	1003.52	Joback Method
cpg	571.04	J/mol×K	965.12	Joback Method
cpg	563.84	J/mol×K	926.71	Joback Method
cpg	555.81	J/mol×K	888.31	Joback Method
cpg	587.71	J/mol×K	1080.33	Joback Method
dvisc	0.0000744	Pa×s	849.90	Joback Method
dvisc	0.0000898	Pa×s	803.53	Joback Method

dvisc	0.0001108	Pa×s	757.16	Joback Method
dvisc	0.0001406	Pa×s	710.80	Joback Method
dvisc	0.0001844	Pa×s	664.43	Joback Method
dvisc	0.0002518	Pa×s	618.06	Joback Method
dvisc	0.0003618	Pa×s	571.69	Joback Method

Sources

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=U348240&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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