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

Inchi: InChI=1S/C15H14Cl4O4/c1-2-3-4-7-22-11(20)5-6-12(21)23-10-8-9(16)13(17)15(19)14(10

InchiKey: DCJDIWNEHHPQNL-AATRIKPKSA-N

Formula: C15H14Cl4O4

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

Mol. weight [g/mol]: 400.08

Physical Properties

Property code	Value	Unit	Source
gf	-286.03	kJ/mol	Joback Method
hf	-597.62	kJ/mol	Joback Method
hfus	49.65	kJ/mol	Joback Method
hvap	89.72	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.495		Crippen Method
mcvol	257.990	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2678.00		NIST Webbook
tb	895.66	K	Joback Method
tc	1121.83	K	Joback Method
tf	594.23	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.59	J/mol×K	895.66	Joback Method
cpg	665.24	J/mol×K	933.36	Joback Method
cpg	673.96	J/mol×K	971.05	Joback Method
cpg	681.78	J/mol×K	1008.75	Joback Method
cpg	688.71	J/mol×K	1046.44	Joback Method
cpg	694.76	J/mol×K	1084.14	Joback Method
cpg	699.95	J/mol×K	1121.83	Joback Method
dvisc	0.0002987	Pa×s	594.23	Joback Method
dvisc	0.0002029	Pa×s	644.47	Joback Method

dvisc	0.0001457	Pa×s	694.71	Joback Method
dvisc	0.0001094	Pa×s	744.95	Joback Method
dvisc	0.0000852	Pa×s	795.18	Joback Method
dvisc	0.0000684	Pa×s	845.42	Joback Method
dvisc	0.0000562	Pa×s	895.66	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=U348243&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