

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

Inchi:	InChI=1S/C13H10Cl4O4/c1-2-5-20-9(18)3-4-10(19)21-13-8(15)6-7(14)11(16)12(13)17/h3
InchiKey:	YZQJZHDNIAAPNN-ONEGZZNKSA-N
Formula:	C13H10Cl4O4
SMILES:	CCCOC(=O)C=CC(=O)Oc1c(Cl)cc(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
rinqol	2385.00		NIST Webbook
tb	849.90	K	Joback Method
tc	1080.33	K	Joback Method
tf	571.69	K	Joback Method
vc	0.879	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.94	J/molxK	849.90	Joback Method
cpg	555.81	J/molxK	888.31	Joback Method
cpg	563.84	J/molxK	926.71	Joback Method
cpg	571.04	J/molxK	965.12	Joback Method
cpg	577.41	J/molxK	1003.52	Joback Method
cpg	582.97	J/molxK	1041.93	Joback Method
cpg	587.71	J/molxK	1080.33	Joback Method
dvisc	0.0003618	Paxs	571.69	Joback Method
dvisc	0.0002518	Paxs	618.06	Joback Method

dvisc	0.0001844	Paxs	664.43	Joback Method
dvisc	0.0001406	Paxs	710.80	Joback Method
dvisc	0.0001108	Paxs	757.16	Joback Method
dvisc	0.0000898	Paxs	803.53	Joback Method
dvisc	0.0000744	Paxs	849.90	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=U348193&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

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