

Fumaric acid, ethyl 2,3,5,6-tetrachlorophenyl ester

Inchi:	InChI=1S/C12H8Cl4O4/c1-2-19-8(17)3-4-9(18)20-12-10(15)6(13)5-7(14)11(12)16/h3-5H
InchiKey:	SCTMAYQQQLGGGL-ONEGZZNKSA-N
Formula:	C12H8Cl4O4
SMILES:	CCOC(=O)C=CC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	358.00

Physical Properties

Property code	Value	Unit	Source
gf	-311.29	kJ/mol	Joback Method
hf	-535.70	kJ/mol	Joback Method
hfus	41.88	kJ/mol	Joback Method
hvap	83.04	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.325		Crippen Method
mvol	215.720	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rmpol	2272.00		NIST Webbook
tb	827.02	K	Joback Method
tc	1060.57	K	Joback Method
tf	560.42	K	Joback Method
vc	0.824	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.07	J/molxK	827.02	Joback Method
cpg	528.08	J/molxK	1021.64	Joback Method
cpg	522.86	J/molxK	982.72	Joback Method
cpg	516.85	J/molxK	943.79	Joback Method
cpg	510.05	J/molxK	904.87	Joback Method
cpg	502.46	J/molxK	865.94	Joback Method
cpg	532.52	J/molxK	1060.57	Joback Method
dvisc	0.0000853	Paxs	827.02	Joback Method
dvisc	0.0001025	Paxs	782.59	Joback Method

dvisc	0.0001258	Paxs	738.15	Joback Method
dvisc	0.0001586	Paxs	693.72	Joback Method
dvisc	0.0002063	Paxs	649.29	Joback Method
dvisc	0.0002790	Paxs	604.85	Joback Method
dvisc	0.0003957	Paxs	560.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348246&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mvol:	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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