

Fumaric acid, 2,6-dimethoxyphenyl 2,3-dichlorophenyl ester

Inchi:	InChI=1S/C18H14Cl2O6/c1-23-13-7-4-8-14(24-2)18(13)26-16(22)10-9-15(21)25-12-6-3-5
InchiKey:	DWNMKDCLMZJUPB-MDZDMXLPSA-N
Formula:	C18H14Cl2O6
SMILES:	COc1cccc(OC)c1OC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	397.21

Physical Properties

Property code	Value	Unit	Source
gf	-334.50	kJ/mol	Joback Method
hf	-655.97	kJ/mol	Joback Method
hfus	45.45	kJ/mol	Joback Method
hvap	94.72	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.078		Crippen Method
mvol	263.760	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
tb	960.96	K	Joback Method
tc	1201.07	K	Joback Method
tf	639.08	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.08	J/molxK	960.96	Joback Method
cpg	758.10	J/molxK	1161.05	Joback Method
cpg	754.97	J/molxK	1121.03	Joback Method
cpg	750.40	J/molxK	1081.01	Joback Method
cpg	744.39	J/molxK	1041.00	Joback Method
cpg	736.95	J/molxK	1000.98	Joback Method
cpg	759.77	J/molxK	1201.07	Joback Method
dvisc	0.0000288	Paxs	960.96	Joback Method
dvisc	0.0000350	Paxs	907.31	Joback Method
dvisc	0.0000435	Paxs	853.67	Joback Method

dvisc	0.0000558	Paxs	800.02	Joback Method
dvisc	0.0000742	Paxs	746.37	Joback Method
dvisc	0.0001031	Paxs	692.73	Joback Method
dvisc	0.0001513	Paxs	639.08	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=U405761&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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