Fumaric acid, 2,6-dimethoxyphenyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C14H14Cl2O6/c1-19-9-4-3-5-10(20-2)14(9)22-13(18)7-6-12(17)21-8-11(15)16/

InchiKey: HLTRWFDYVVWERS-VOTSOKGWSA-N

Formula: C14H14Cl2O6

SMILES: COc1cccc(OC)c1OC(=O)C=CC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 349.16

Physical Properties

Property code	Value	Unit	Source
gf	-463.77	kJ/mol	Joback Method
hf	-792.28	kJ/mol	Joback Method
hfus	38.30	kJ/mol	Joback Method
hvap	81.83	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.512		Crippen Method
mcvol	231.160	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	2389.00		NIST Webbook
rinpol	2389.00		NIST Webbook
tb	832.36	K	Joback Method
tc	1052.66	K	Joback Method
tf	527.54	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.14	J/mol×K	832.36	Joback Method
cpg	625.09	J/mol×K	869.08	Joback Method
cpg	635.00	J/mol×K	905.79	Joback Method
cpg	643.84	J/mol×K	942.51	Joback Method
cpg	651.61	J/mol×K	979.22	Joback Method
cpg	658.30	J/mol×K	1015.94	Joback Method
cpg	663.89	J/mol×K	1052.66	Joback Method
dvisc	0.0003253	Pa×s	527.54	Joback Method

dvisc	0.0002008	Pa×s	578.34	Joback Method
dvisc	0.0001340	Pa×s	629.15	Joback Method
dvisc	0.0000950	Pa×s	679.95	Joback Method
dvisc	0.0000706	Pa×s	730.75	Joback Method
dvisc	0.0000546	Pa×s	781.56	Joback Method
dvisc	0.0000435	Pa×s	832.36	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=U405752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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