

Fumaric acid, 4-chlorophenyl 3-chlorophenyl ester

Inchi:	InChI=1S/C16H10Cl2O4/c17-11-4-6-13(7-5-11)21-15(19)8-9-16(20)22-14-3-1-2-12(18)10
InchiKey:	JFCKNIYTEHGGNK-CMDGGOBGSA-N
Formula:	C16H10Cl2O4
SMILES:	O=C(C=CC(=O)Oc1cccc(Cl)c1)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	337.15

Physical Properties

Property code	Value	Unit	Source
gf	-122.08	kJ/mol	Joback Method
hf	-327.31	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Joback Method
hvap	84.13	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.061		Crippen Method
mcvol	223.840	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rmpol	2528.00		NIST Webbook
tb	860.40	K	Joback Method
tc	1109.51	K	Joback Method
tf	547.04	K	Joback Method
vc	0.842	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.70	J/molxK	860.40	Joback Method
cpg	613.08	J/molxK	1067.99	Joback Method
cpg	607.01	J/molxK	1026.48	Joback Method
cpg	599.99	J/molxK	984.96	Joback Method
cpg	591.97	J/molxK	943.44	Joback Method
cpg	582.89	J/molxK	901.92	Joback Method
cpg	618.25	J/molxK	1109.51	Joback Method
dvisc	0.0000653	Paxs	860.40	Joback Method
dvisc	0.0000808	Paxs	808.17	Joback Method

dvisc	0.0001030	Paxs	755.95	Joback Method
dvisc	0.0001361	Paxs	703.72	Joback Method
dvisc	0.0001880	Paxs	651.49	Joback Method
dvisc	0.0002747	Paxs	599.27	Joback Method
dvisc	0.0004317	Paxs	547.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405845&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

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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