

Fumaric acid, 4-chlorophenyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C16H8Cl4O4/c17-9-1-3-11(4-2-9)23-14(21)5-6-15(22)24-16-12(19)7-10(18)8-1
InchiKey:	YTZAOGZOZASQRM-AATRIKPKSA-N
Formula:	C16H8Cl4O4
SMILES:	O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	406.04

Physical Properties

Property code	Value	Unit	Source
gf	-165.20	kJ/mol	Joback Method
hf	-381.73	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	94.22	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.367		Crippen Method
mcvol	248.320	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	2799.00		NIST Webbook
rinpol	2799.00		NIST Webbook
tb	945.22	K	Joback Method
tc	1199.71	K	Joback Method
tf	631.92	K	Joback Method
vc	0.940	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.57	J/molxK	945.22	Joback Method
cpg	631.19	J/molxK	1157.30	Joback Method
cpg	627.60	J/molxK	1114.88	Joback Method
cpg	623.09	J/molxK	1072.47	Joback Method
cpg	617.60	J/molxK	1030.05	Joback Method
cpg	611.11	J/molxK	987.64	Joback Method
cpg	633.89	J/molxK	1199.71	Joback Method
dvisc	0.0000506	Paxs	945.22	Joback Method

dvisc	0.0000612	Paxs	893.00	Joback Method
dvisc	0.0000758	Paxs	840.79	Joback Method
dvisc	0.0000965	Paxs	788.57	Joback Method
dvisc	0.0001273	Paxs	736.35	Joback Method
dvisc	0.0001751	Paxs	684.14	Joback Method
dvisc	0.0002539	Paxs	631.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405848&Units=SI

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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