

Fumaric acid, 2,4-dichlorophenyl 3-chlorophenyl ester

Inchi:	InChI=1S/C16H9Cl3O4/c17-10-2-1-3-12(8-10)22-15(20)6-7-16(21)23-14-5-4-11(18)9-13
InchiKey:	MHYBGCKFTSIVKJ-VOTSOKGWSA-N
Formula:	C16H9Cl3O4
SMILES:	O=C(C=CC(=O)Oc1ccc(Cl)cc1Cl)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	371.60

Physical Properties

Property code	Value	Unit	Source
gf	-143.64	kJ/mol	Joback Method
hf	-354.52	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.714		Crippen Method
mcvol	236.080	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	2643.00		NIST Webbook
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tb	902.81	K	Joback Method
tc	1154.56	K	Joback Method
tf	589.48	K	Joback Method
vc	0.890	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.02	J/molxK	902.81	Joback Method
cpg	597.86	J/molxK	944.77	Joback Method
cpg	605.64	J/molxK	986.73	Joback Method
cpg	612.39	J/molxK	1028.69	Joback Method
cpg	618.16	J/molxK	1070.65	Joback Method
cpg	622.99	J/molxK	1112.60	Joback Method
cpg	626.94	J/molxK	1154.56	Joback Method
dvisc	0.0003288	Paxs	589.48	Joback Method

dvisc	0.0002186	Paxs	641.70	Joback Method
dvisc	0.0001545	Paxs	693.92	Joback Method
dvisc	0.0001147	Paxs	746.14	Joback Method
dvisc	0.0000885	Paxs	798.37	Joback Method
dvisc	0.0000705	Paxs	850.59	Joback Method
dvisc	0.0000577	Paxs	902.81	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=U405701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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