

Fumaric acid, ethyl 2,3,6-trichlorophenyl ester

Inchi:	InChI=1S/C12H9Cl3O4/c1-2-18-9(16)5-6-10(17)19-12-8(14)4-3-7(13)11(12)15/h3-6H,2H
InchiKey:	VXWLCYIYNUHENI-AATRIKPKSA-N
Formula:	C12H9Cl3O4
SMILES:	CCOC(=O)C=CC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	323.56

Physical Properties

Property code	Value	Unit	Source
gf	-289.73	kJ/mol	Joback Method
hf	-508.49	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	77.99	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.671		Crippen Method
mcvol	203.480	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinsol	2138.00		NIST Webbook
tb	784.61	K	Joback Method
tc	1014.85	K	Joback Method
tf	517.98	K	Joback Method
vc	0.774	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.14	J/molxK	784.61	Joback Method
cpg	516.55	J/molxK	976.48	Joback Method
cpg	510.23	J/molxK	938.11	Joback Method
cpg	503.14	J/molxK	899.73	Joback Method
cpg	495.27	J/molxK	861.36	Joback Method
cpg	486.61	J/molxK	822.98	Joback Method
cpg	522.10	J/molxK	1014.85	Joback Method
dvisc	0.0000962	Paxs	784.61	Joback Method
dvisc	0.0001169	Paxs	740.17	Joback Method

dvisc	0.0001457	Paxs	695.73	Joback Method
dvisc	0.0001870	Paxs	651.30	Joback Method
dvisc	0.0002490	Paxs	606.86	Joback Method
dvisc	0.0003469	Paxs	562.42	Joback Method
dvisc	0.0005116	Paxs	517.98	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=U348219&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

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