

Fumaric acid, di(2-chloropropyl) ester

Inchi:	InChI=1S/C10H14Cl2O4/c1-7(11)5-15-9(13)3-4-10(14)16-6-8(2)12/h3-4,7-8H,5-6H2,1-2H
InchiKey:	XTVLIWMGYKFLMA-ONEGZZNKSA-N
Formula:	C10H14Cl2O4
SMILES:	CC(Cl)COC(=O)C=CC(=O)OCC(C)Cl
Mol. weight [g/mol]:	269.12

Physical Properties

Property code	Value	Unit	Source
gf	-383.04	kJ/mol	Joback Method
hf	-664.15	kJ/mol	Joback Method
hfus	28.78	kJ/mol	Joback Method
hvap	64.12	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.884		Crippen Method
mcvol	186.820	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinsol	1766.00		NIST Webbook
tb	658.92	K	Joback Method
tc	861.17	K	Joback Method
tf	371.54	K	Joback Method
vc	0.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.61	J/molxK	658.92	Joback Method
cpg	460.35	J/molxK	692.63	Joback Method
cpg	471.41	J/molxK	726.34	Joback Method
cpg	481.80	J/molxK	760.05	Joback Method
cpg	491.54	J/molxK	793.76	Joback Method
cpg	500.62	J/molxK	827.47	Joback Method
cpg	509.06	J/molxK	861.17	Joback Method
dvisc	0.0019525	Paxs	371.54	Joback Method
dvisc	0.0009386	Paxs	419.44	Joback Method

dvisc	0.0005243	Paxs	467.33	Joback Method
dvisc	0.0003264	Paxs	515.23	Joback Method
dvisc	0.0002202	Paxs	563.13	Joback Method
dvisc	0.0001580	Paxs	611.02	Joback Method
dvisc	0.0001190	Paxs	658.92	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=U348573&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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