Fumaric acid, di(2,2-dichloroethyl) ester

Inchi: InChI=1S/C8H8Cl4O4/c9-5(10)3-15-7(13)1-2-8(14)16-4-6(11)12/h1-2,5-6H,3-4H2/b2-1+
InchiKey: FSRFBNQOJOZBHW-OWOJBTEDSA-N
Formula: C8H8Cl4O4
SMILES: O=C(C=CC(=O)OCC(Cl)Cl)OCC(Cl)Cl
Mol. weight [g/mol]: 309.96

Physical Properties

Property code	Value	Unit	Source
gf	-423.74	kJ/mol	Joback Method
hf	-654.35	kJ/mol	Joback Method
hfus	31.99	kJ/mol	Joback Method
hvap	68.44	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.236		Crippen Method
mcvol	183.120	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1874.00		NIST Webbook
tb	688.02	K	Joback Method
tc	903.13	K	Joback Method
tf	408.84	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.29	J/mol×K	688.02	Joback Method
cpg	403.94	J/mol×K	723.87	Joback Method
cpg	411.97	J/mol×K	759.72	Joback Method
cpg	419.39	J/mol×K	795.58	Joback Method
cpg	426.22	J/mol×K	831.43	Joback Method
cpg	432.46	J/mol×K	867.28	Joback Method
cpg	438.13	J/mol×K	903.13	Joback Method
dvisc	0.0015108	Pa×s	408.84	Joback Method
dvisc	0.0008013	Pa×s	455.37	Joback Method

dvisc	0.0004780	Pa×s	501.90	Joback Method
dvisc	0.0003113	Pa×s	548.43	Joback Method
dvisc	0.0002168	Pa×s	594.96	Joback Method
dvisc	0.0001591	Pa×s	641.49	Joback Method
dvisc	0.0001218	Pa×s	688.02	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=U348583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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