Fumaric acid, 2,2-dichloroethyl isobutyl ester

Inchi: InChI=1S/C10H14Cl2O4/c1-7(2)5-15-9(13)3-4-10(14)16-6-8(11)12/h3-4,7-8H,5-6H2,1-2H
InchiKey: IKJKPEUGXREZPB-ONEGZZNKSA-N
Formula: C10H14Cl2O4
SMILES: CC(C)COC(=O)C=CC(=O)OCC(Cl)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	-2.26		Crippen Method
logp	2.089		Crippen Method
mcvol	186.820	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
tb	658.92	K	Joback Method
tc	861.17	K	Joback Method
tf	371.54	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.61	J/mol×K	658.92	Joback Method
cpg	460.35	J/mol×K	692.63	Joback Method
cpg	471.41	J/mol×K	726.34	Joback Method
cpg	481.80	J/mol×K	760.05	Joback Method
cpg	491.54	J/mol×K	793.76	Joback Method
cpg	500.62	J/mol×K	827.47	Joback Method
cpg	509.06	J/mol×K	861.17	Joback Method
dvisc	0.0019525	Pa×s	371.54	Joback Method

dvisc	0.0009386	Pa×s	419.44	Joback Method
dvisc	0.0005243	Pa×s	467.33	Joback Method
dvisc	0.0003264	Pa×s	515.23	Joback Method
dvisc	0.0002202	Pa×s	563.13	Joback Method
dvisc	0.0001580	Pa×s	611.02	Joback Method
dvisc	0.0001190	Pa×s	658.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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