Fumaric acid, monochloride, pent-4-en-2-yl ester

Other names: Fumaric acid, monochloride, pent-4-en-2-yl chloride
Inchi: InChI=1S/C9H11ClO3/c1-3-4-7(2)13-9(12)6-5-8(10)11/h3,5-7H,1,4H2,2H3/b6-5+
InchiKey: WBAFEBVXXKAFFY-AATRIKPKSA-N
Formula: C9H11ClO3
SMILES: C=CCC(C)OC(=O)C=CC(=O)Cl
Mol. weight [g/mol]: 202.63

Physical Properties

Property code	Value	Unit	Source
gf	-184.25	kJ/mol	Joback Method
hf	-364.84	kJ/mol	Joback Method
hfus	23.05	kJ/mol	Joback Method
hvap	54.81	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.816		Crippen Method
mcvol	150.320	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
tb	573.31	K	Joback Method
tc	776.30	K	Joback Method
tf	321.36	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.27	J/mol×K	573.31	Joback Method
cpg	380.16	J/mol×K	742.47	Joback Method
cpg	371.54	J/mol×K	708.64	Joback Method
cpg	362.36	J/mol×K	674.80	Joback Method
cpg	352.61	J/mol×K	640.97	Joback Method
cpg	342.25	J/mol×K	607.14	Joback Method
cpg	388.25	J/mol×K	776.30	Joback Method

dvisc	0.0002064	Pa×s	573.31	Joback Method
dvisc	0.0002680	Pa×s	531.32	Joback Method
dvisc	0.0003638	Pa×s	489.33	Joback Method
dvisc	0.0005231	Pa×s	447.33	Joback Method
dvisc	0.0008108	Pa×s	405.34	Joback Method
dvisc	0.0013907	Pa×s	363.35	Joback Method
dvisc	0.0027468	Pa×s	321.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348935&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