Fumaric acid, propyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C9H11Cl3O4/c1-2-5-15-7(13)3-4-8(14)16-6-9(10,11)12/h3-4H,2,5-6H2,1H3/b4
InchiKey: GQQOPVNABGMTHV-ONEGZZNKSA-N
Formula: C9H11Cl3O4
SMILES: CCCOC(=O)C=CC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 289.54

Physical Properties

Property code	Value	Unit	Source
gf	-395.67	kJ/mol	Joback Method
hf	-657.44	kJ/mol	Joback Method
hfus	30.02	kJ/mol	Joback Method
hvap	65.76	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.409		Crippen Method
mcvol	184.970	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1659.00		NIST Webbook
tb	671.12	K	Joback Method
tc	882.92	K	Joback Method
tf	422.61	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.91	J/mol×K	671.12	Joback Method
cpg	468.51	J/mol×K	847.62	Joback Method
cpg	461.06	J/mol×K	812.32	Joback Method
cpg	453.01	J/mol×K	777.02	Joback Method
cpg	444.32	J/mol×K	741.72	Joback Method
cpg	434.97	J/mol×K	706.42	Joback Method
cpg	475.37	J/mol×K	882.92	Joback Method
dvisc	0.0001199	Pa×s	671.12	Joback Method
dvisc	0.0001550	Pa×s	629.70	Joback Method

dvisc	0.0002079	Pa×s	588.28	Joback Method
dvisc	0.0002916	Pa×s	546.87	Joback Method
dvisc	0.0004321	Pa×s	505.45	Joback Method
dvisc	0.0006869	Pa×s	464.03	Joback Method
dvisc	0.0011959	Pa×s	422.61	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=U348501&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