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

Inchi: InChI=1S/C8H6Cl6O4/c9-7(10,11)3-17-5(15)1-2-6(16)18-4-8(12,13)14/h1-2H,3-4H2/b2-1
InchiKey: WFTACGQPAJJUOO-OWOJBTEDSA-N
Formula: C8H6Cl6O4
SMILES: O=C(C=CC(=O)OCC(Cl)(Cl)Cl)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 378.85

Physical Properties

Property code	Value	Unit	Source
gf	-437.04	kJ/mol	Joback Method
hf	-692.77	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	75.39	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.369		Crippen Method
mcvol	207.600	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1997.00		NIST Webbook
tb	757.30	K	Joback Method
tc	993.10	K	Joback Method
tf	503.52	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.47	J/mol×K	757.30	Joback Method
cpg	444.08	J/mol×K	796.60	Joback Method
cpg	450.01	J/mol×K	835.90	Joback Method
cpg	455.34	J/mol×K	875.20	Joback Method
cpg	460.13	J/mol×K	914.50	Joback Method
cpg	464.47	J/mol×K	953.80	Joback Method
cpg	468.41	J/mol×K	993.10	Joback Method
dvisc	0.0006338	Pa×s	503.52	Joback Method
dvisc	0.0003823	Pa×s	545.82	Joback Method

dvisc	0.0002479	Pa×s	588.11	Joback Method
dvisc	0.0001704	Pa×s	630.41	Joback Method
dvisc	0.0001228	Pa×s	672.71	Joback Method
dvisc	0.0000920	Pa×s	715.00	Joback Method
dvisc	0.0000712	Pa×s	757.30	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U348511&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