Propanoic acid, pentachloro-, methyl ester

Other names: Methyl pentachloro-propanoate
Inchi: InChI=1S/C4H3Cl5O2/c1-11-2(10)3(5,6)4(7,8)9/h1H3
InchiKey: YSCHNGJMUJYQJG-UHFFFAOYSA-N
Formula: C4H3Cl5O2
SMILES: COC(=O)C(Cl)(Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 260.33
CAS: 813-46-7

Physical Properties

Property code	Value	Unit	Source
gf	-305.09	kJ/mol	Joback Method
hf	-466.89	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	52.99	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.703		Crippen Method
mcvol	135.860	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1275.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1275.00		NIST Webbook
tb	547.90	K	Joback Method
tc	787.31	K	Joback Method
tf	361.44	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.96	J/mol×K	547.90	Joback Method
cpg	244.16	J/mol×K	587.80	Joback Method
cpg	249.65	J/mol×K	627.70	Joback Method

cpg	254.48	J/mol×K	667.61	Joback Method
cpg	258.72	J/mol×K	707.51	Joback Method
cpg	262.43	J/mol×K	747.41	Joback Method
cpg	265.66	J/mol×K	787.31	Joback Method
dvisc	0.0026580	Pa×s	361.44	Joback Method
dvisc	0.0015736	Pa×s	392.52	Joback Method
dvisc	0.0010061	Pa×s	423.59	Joback Method
dvisc	0.0006838	Pa×s	454.67	Joback Method
dvisc	0.0004883	Pa×s	485.75	Joback Method
dvisc	0.0003631	Pa×s	516.82	Joback Method
dvisc	0.0002793	Pa×s	547.90	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=C813467&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