Acetic acid, trichloro-, 1,1-dimethylethyl ester

Inchi: InChI=1S/C6H9Cl3O2/c1-5(2,3)11-4(10)6(7,8)9/h1-3H3
InchiKey: YROVKSCEXQTHTJ-UHFFFAOYSA-N
Formula: C6H9Cl3O2
SMILES: CC(C)(C)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 219.49
CAS: 1860-21-5

Physical Properties

Property code	Value	Unit	Source
gf	-264.39	kJ/mol	Joback Method
hf	-476.69	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	48.67	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.698		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
ripol	1315.00		NIST Webbook
ripol	1315.00		NIST Webbook
tb	518.80	K	Joback Method
tc	740.23	K	Joback Method
tf	324.14	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.39	J/mol×K	518.80	Joback Method
cpg	289.68	J/mol×K	555.70	Joback Method
cpg	299.15	J/mol×K	592.61	Joback Method
cpg	307.85	J/mol×K	629.51	Joback Method
cpg	315.85	J/mol×K	666.42	Joback Method

cpg	323.18	J/mol×K	703.32	Joback Method
cpg	329.90	J/mol×K	740.23	Joback Method
dvisc	0.0036065	Pa×s	324.14	Joback Method
dvisc	0.0019239	Pa×s	356.58	Joback Method
dvisc	0.0011397	Pa×s	389.03	Joback Method
dvisc	0.0007318	Pa×s	421.47	Joback Method
dvisc	0.0005006	Pa×s	453.91	Joback Method
dvisc	0.0003603	Pa×s	486.36	Joback Method
dvisc	0.0002702	Pa×s	518.80	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1860215&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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