Trichloroacetic acid, 2-butyl ester

Other names: Acetic acid, trichloro, 1-methylpropyl ester
Inchi: InChI=1S/C6H9Cl3O2/c1-3-4(2)11-5(10)6(7,8)9/h4H,3H2,1-2H3
InchiKey: CJTKROHEGUUXOZ-UHFFFAOYSA-N
Formula: C6H9Cl3O2
SMILES: CCC(C)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 219.49
CAS: 4484-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-269.67	kJ/mol	Joback Method
hf	-473.22	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.698		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook
ripol	1395.00		NIST Webbook
tb	521.59	K	Joback Method
tc	734.09	K	Joback Method
tf	306.72	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.03	J/mol×K	521.59	Joback Method
cpg	285.82	J/mol×K	557.01	Joback Method
cpg	294.97	J/mol×K	592.42	Joback Method
cpg	303.52	J/mol×K	627.84	Joback Method
cpg	311.49	J/mol×K	663.25	Joback Method

cpg	318.90	J/mol×K	698.67	Joback Method
cpg	325.79	J/mol×K	734.09	Joback Method
dvisc	0.0041126	Pa×s	306.72	Joback Method
dvisc	0.0020546	Pa×s	342.53	Joback Method
dvisc	0.0011705	Pa×s	378.34	Joback Method
dvisc	0.0007350	Pa×s	414.16	Joback Method
dvisc	0.0004970	Pa×s	449.97	Joback Method
dvisc	0.0003560	Pa×s	485.78	Joback Method
dvisc	0.0002670	Pa×s	521.59	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=C4484804&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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