2-Butanone, 1,1,3-trichloro

Inchi: InChI=1S/C4H5Cl3O/c1-2(5)3(8)4(6)7/h2,4H,1H3
InchiKey: QTGXVEKFZMQAHV-UHFFFAOYSA-N
Formula: C4H5Cl3O
SMILES: CC(Cl)C(=O)C(Cl)Cl
Mol. weight [g/mol]: 175.44

Physical Properties

Property code	Value	Unit	Source
gf	-186.79	kJ/mol	Joback Method
hf	-296.25	kJ/mol	Joback Method
hfus	13.26	kJ/mol	Joback Method
hvap	43.62	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.987		Crippen Method
mcvol	105.510	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
rinpol	971.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	956.00		NIST Webbook
tb	456.20	K	Joback Method
tc	668.15	K	Joback Method
tf	244.53	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.49	J/mol×K	456.20	Joback Method
cpg	180.34	J/mol×K	491.53	Joback Method
cpg	186.79	J/mol×K	526.85	Joback Method
cpg	192.83	J/mol×K	562.18	Joback Method

cpg	198.50	J/mol×K	597.50	Joback Method
cpg	203.80	J/mol×K	632.83	Joback Method
cpg	208.74	J/mol×K	668.15	Joback Method
dvisc	0.0071264	Pa×s	244.53	Joback Method
dvisc	0.0032499	Pa×s	279.81	Joback Method
dvisc	0.0017669	Pa×s	315.09	Joback Method
dvisc	0.0010861	Pa×s	350.37	Joback Method
dvisc	0.0007298	Pa×s	385.64	Joback Method
dvisc	0.0005241	Pa×s	420.92	Joback Method
dvisc	0.0003962	Pa×s	456.20	Joback Method

Sources

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=R629439&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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