

3-Buten-1-ol, trichloroacetate

Inchi:	InChI=1S/C6H7Cl3O2/c1-2-3-4-11-5(10)6(7,8)9/h2H,1,3-4H2
InchiKey:	JNUGOAAJACV GAL-UHFFFAOYSA-N
Formula:	C6H7Cl3O2
SMILES:	C=CCCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	217.48

Physical Properties

Property code	Value	Unit	Source
gf	-179.39	kJ/mol	Joback Method
hf	-342.51	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	49.30	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.476		Crippen Method
mcvol	135.260	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1122.00		NIST Webbook
ripol	1546.00		NIST Webbook
tb	518.71	K	Joback Method
tc	731.04	K	Joback Method
tf	319.96	K	Joback Method
vc	0.512	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.64	J/molxK	518.71	Joback Method
cpg	266.35	J/molxK	554.10	Joback Method
cpg	274.45	J/molxK	589.49	Joback Method
cpg	281.98	J/molxK	624.88	Joback Method
cpg	288.96	J/molxK	660.26	Joback Method
cpg	295.43	J/molxK	695.65	Joback Method
cpg	301.41	J/molxK	731.04	Joback Method
dvisc	0.0029426	Paxs	319.96	Joback Method

dvisc	0.0016695	Paxs	353.09	Joback Method
dvisc	0.0010439	Paxs	386.21	Joback Method
dvisc	0.0007030	Paxs	419.34	Joback Method
dvisc	0.0005016	Paxs	452.46	Joback Method
dvisc	0.0003748	Paxs	485.59	Joback Method
dvisc	0.0002907	Paxs	518.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26457&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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