

Trichloroacetic acid, but-3-yn-2-yl ester

Inchi:	InChI=1S/C6H5Cl3O2/c1-3-4(2)11-5(10)6(7,8)9/h1,4H,2H3
InchiKey:	KEBRGWUCOLOSMN-UHFFFAOYSA-N
Formula:	C6H5Cl3O2
SMILES:	C#CC(C)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	215.46

Physical Properties

Property code	Value	Unit	Source
gf	-46.60	kJ/mol	Joback Method
hf	-181.32	kJ/mol	Joback Method
hfus	18.71	kJ/mol	Joback Method
hvap	49.44	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.922		Crippen Method
mcvol	130.960	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	511.71	K	Joback Method
tc	740.24	K	Joback Method
tf	353.69	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.44	J/molxK	511.71	Joback Method
cpg	250.30	J/molxK	549.80	Joback Method
cpg	257.54	J/molxK	587.89	Joback Method
cpg	264.17	J/molxK	625.97	Joback Method
cpg	270.25	J/molxK	664.06	Joback Method
cpg	275.81	J/molxK	702.15	Joback Method
cpg	280.88	J/molxK	740.24	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U299254&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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