2-Propyn-1-ol, tribromoacetate

Inchi: InChI=1S/C5H3Br3O2/c1-2-3-10-4(9)5(6,7)8/h1H,3H2
InchiKey: VSVLPDUZBGOESC-UHFFFAOYSA-N
Formula: C5H3Br3O2
SMILES: C#CCOC(=O)C(Br)(Br)Br
Mol. weight [g/mol]: 334.79

Physical Properties

Property code	Value	Unit	Source
gf	26.17	kJ/mol	Joback Method
hf	-29.19	kJ/mol	Joback Method
hfus	22.91	kJ/mol	Joback Method
hvap	53.75	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.001		Crippen Method
mcvol	132.650	ml/mol	McGowan Method
pc	6122.63	kPa	Joback Method
rinpol	1322.00		NIST Webbook
tb	575.46	K	Joback Method
tc	835.21	K	Joback Method
tf	447.06	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.45	J/mol×K	575.46	Joback Method
cpg	225.91	J/mol×K	618.75	Joback Method
cpg	230.71	J/mol×K	662.04	Joback Method
cpg	234.97	J/mol×K	705.34	Joback Method
cpg	238.74	J/mol×K	748.63	Joback Method
cpg	242.14	J/mol×K	791.92	Joback Method
cpg	245.23	J/mol×K	835.21	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=R26386&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume