Ethyl tribromoacetate

Other names: Acetic acid, 2,2,2-tribromoethyl ester
Inchi: InChI=1S/C4H5Br3O2/c1-2-9-3(8)4(5,6)7/h2H2,1H3
InchiKey: ZZUKBDJWZXVOQG-UHFFFAOYSA-N
Formula: C4H5Br3O2
SMILES: CCOC(=O)C(Br)(Br)Br
Mol. weight [g/mol]: 324.79
CAS: 599-99-5

Physical Properties

Property code	Value	Unit	Source
gf	-205.32	kJ/mol	Joback Method
hf	-300.45	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	51.66	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.388		Crippen Method
mcvol	127.160	ml/mol	McGowan Method
pc	5653.23	kPa	Joback Method
tb	562.46	K	Joback Method
tc	808.56	K	Joback Method
tf	388.82	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.73	J/mol×K	562.46	Joback Method
cpg	242.52	J/mol×K	767.54	Joback Method
cpg	238.16	J/mol×K	726.53	Joback Method
cpg	233.37	J/mol×K	685.51	Joback Method
cpg	228.07	J/mol×K	644.49	Joback Method
cpg	222.21	J/mol×K	603.48	Joback Method
cpg	246.51	J/mol×K	808.56	Joback Method
dvisc	0.0003169	Pa×s	562.46	Joback Method

dvisc	0.0003899	Pa×s	533.52	Joback Method
dvisc	0.0004913	Pa×s	504.58	Joback Method
dvisc	0.0006368	Pa×s	475.64	Joback Method
dvisc	0.0008535	Pa×s	446.70	Joback Method
dvisc	0.0011913	Pa×s	417.76	Joback Method
dvisc	0.0017474	Pa×s	388.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.20	K	9.70	NIST Webbook

Sources

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=C599995&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume