

Tribromoacetic acid, methyl ester

Other names:	Methyl tribromoacetate
Inchi:	InChI=1S/C3H3Br3O2/c1-8-2(7)3(4,5)6/h1H3
InchiKey:	QQHSHLKOWBDOFC-UHFFFAOYSA-N
Formula:	C3H3Br3O2
SMILES:	COC(=O)C(Br)(Br)Br
Mol. weight [g/mol]:	310.77
CAS:	3222-05-7

Physical Properties

Property code	Value	Unit	Source
gf	-213.74	kJ/mol	Joback Method
hf	-279.81	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	49.44	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.998		Crippen Method
mcvol	113.070	ml/mol	McGowan Method
pc	6567.04	kPa	Joback Method
rinpol	1174.00		NIST Webbook
tb	539.58	K	Joback Method
tc	791.04	K	Joback Method
tf	377.55	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.45	J/molxK	539.58	Joback Method
cpg	180.54	J/molxK	581.49	Joback Method
cpg	185.07	J/molxK	623.40	Joback Method
cpg	189.10	J/molxK	665.31	Joback Method
cpg	192.69	J/molxK	707.22	Joback Method
cpg	195.88	J/molxK	749.13	Joback Method
cpg	198.76	J/molxK	791.04	Joback Method

dvisc	0.0018751	Paxs	377.55	Joback Method
dvisc	0.0013036	Paxs	404.56	Joback Method
dvisc	0.0009485	Paxs	431.56	Joback Method
dvisc	0.0007164	Paxs	458.56	Joback Method
dvisc	0.0005583	Paxs	485.57	Joback Method
dvisc	0.0004467	Paxs	512.57	Joback Method
dvisc	0.0003654	Paxs	539.58	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3222057&Units=SI

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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