Methyl tribromoacetate

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

Physical Properties

Property code	Value	Unit	Source
hf	-217.65	kJ/mol	Cheméo Relay (1.0)
hfus	14.75	kJ/mol	Joback Method
hvap	55.33	kJ/mol	Cheméo Relay (1.0)
ie	10.56	eV	Cheméo Relay (1.0)
logp	1.998		Crippen Method
mcvol	113.070	ml/mol	McGowan Method
rinpol	1174.00		NIST Webbook
rinpol	1174.00		NIST Webbook
tb	485.27	K	Cheméo Relay (1.0)
tf	264.85	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.45	J/mol×K	539.58	Joback Method
cpg	180.54	J/mol×K	581.49	Joback Method
cpg	185.07	J/mol×K	623.40	Joback Method
cpg	189.10	J/mol×K	665.31	Joback Method
cpg	192.69	J/mol×K	707.22	Joback Method
cpg	195.88	J/mol×K	749.13	Joback Method
cpg	198.76	J/mol×K	791.04	Joback Method
dvisc	0.0018751	Pa×s	377.55	Joback Method
dvisc	0.0013036	Pa×s	404.56	Joback Method
dvisc	0.0009485	Pa×s	431.56	Joback Method
dvisc	0.0007164	Pa×s	458.56	Joback Method

dvisc	0.0005583	Pa×s	485.57	Joback Method
dvisc	0.0004467	Pa×s	512.57	Joback Method
dvisc	0.0003654	Pa×s	539.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3222057&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point