

Isopropyl tribromoacetate

Inchi:	InChI=1S/C5H7Br3O2/c1-3(2)10-4(9)5(6,7)8/h3H,1-2H3
InchiKey:	CBISLYVFYBAQAD-UHFFFAOYSA-N
Formula:	C5H7Br3O2
SMILES:	CC(C)OC(=O)C(Br)(Br)Br
Mol. weight [g/mol]:	338.82

Physical Properties

Property code	Value	Unit	Source
gf	-199.34	kJ/mol	Joback Method
hf	-326.37	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.776		Crippen Method
mcvol	141.250	ml/mol	McGowan Method
pc	4973.33	kPa	Joback Method
rinpol	1259.00		NIST Webbook
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tb	584.90	K	Joback Method
tc	831.33	K	Joback Method
tf	385.09	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.37	J/molxK	584.90	Joback Method
cpg	266.30	J/molxK	625.97	Joback Method
cpg	273.53	J/molxK	667.04	Joback Method
cpg	280.11	J/molxK	708.11	Joback Method
cpg	286.10	J/molxK	749.18	Joback Method
cpg	291.59	J/molxK	790.26	Joback Method
cpg	296.63	J/molxK	831.33	Joback Method
dvisc	0.0019419	Paxs	385.09	Joback Method

dvisc	0.0012116	Paxs	418.39	Joback Method
dvisc	0.0008104	Paxs	451.69	Joback Method
dvisc	0.0005729	Paxs	485.00	Joback Method
dvisc	0.0004234	Paxs	518.30	Joback Method
dvisc	0.0003246	Paxs	551.60	Joback Method
dvisc	0.0002564	Paxs	584.90	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=R115881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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