

2-Propanol, 1,1,3-tribromo-

Inchi:	InChI=1S/C3H5Br3O/c4-1-2(7)3(5)6/h2-3,7H,1H2
InchiKey:	QDJVPMNYRGTTFU-UHFFFAOYSA-N
Formula:	C3H5Br3O
SMILES:	OC(CBr)C(Br)Br
Mol. weight [g/mol]:	296.78
CAS:	59228-00-1

Physical Properties

Property code	Value	Unit	Source
gf	-124.36	kJ/mol	Joback Method
hf	-189.05	kJ/mol	Joback Method
hfus	16.42	kJ/mol	Joback Method
hvap	57.48	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.858		Crippen Method
mcvol	111.500	ml/mol	McGowan Method
pc	7049.79	kPa	Joback Method
tb	557.82	K	Joback Method
tc	778.60	K	Joback Method
tf	333.79	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.29	J/molxK	557.82	Joback Method
cpg	184.24	J/molxK	594.62	Joback Method
cpg	188.78	J/molxK	631.41	Joback Method
cpg	192.96	J/molxK	668.21	Joback Method
cpg	196.82	J/molxK	705.00	Joback Method
cpg	200.40	J/molxK	741.80	Joback Method
cpg	203.74	J/molxK	778.60	Joback Method
dvisc	0.0083055	Paxs	333.79	Joback Method
dvisc	0.0031255	Paxs	371.13	Joback Method

dvisc	0.0014063	Paxs	408.47	Joback Method
dvisc	0.0007233	Paxs	445.80	Joback Method
dvisc	0.0004123	Paxs	483.14	Joback Method
dvisc	0.0002548	Paxs	520.48	Joback Method
dvisc	0.0001679	Paxs	557.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59228001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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