

Ethanol, 2,2,2-tribromo-

Other names:	«beta»-Tribromoethanol Avertin Basibrol Bromethol Ethobrom Ethobrome Narcolan Narcotyl Narkolan Rectanol Tribromoethanol 2,2,2-Tribromoethanol 2,2,2-Tribromoethyl alcohol «beta»-Tribromoethyl alcohol Tribromethanol Tribromoethyl alcohol NSC 2189
Inchi:	InChI=1S/C2H3Br3O/c3-2(4,5)1-6/h6H,1H2
InchiKey:	YFDS DPIBEUFTMI-UHFFFAOYSA-N
Formula:	C2H3Br3O
SMILES:	OCC(Br)(Br)Br
Mol. weight [g/mol]:	282.76
CAS:	75-80-9

Physical Properties

Property code	Value	Unit	Source
gf	-125.06	kJ/mol	Joback Method
hf	-166.60	kJ/mol	Joback Method
hfus	13.47	kJ/mol	Joback Method
hvap	54.73	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.817		Crippen Method
mcvol	97.410	ml/mol	McGowan Method
pc	8386.00	kPa	Joback Method
tb	532.59	K	Joback Method
tc	761.69	K	Joback Method
tf	354.94	K	Joback Method

vc	0.342	m ³ /kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.30	J/mol×K	532.59	Joback Method
cpg	146.91	J/mol×K	570.77	Joback Method
cpg	150.04	J/mol×K	608.96	Joback Method
cpg	152.75	J/mol×K	647.14	Joback Method
cpg	155.12	J/mol×K	685.32	Joback Method
cpg	157.20	J/mol×K	723.50	Joback Method
cpg	159.07	J/mol×K	761.69	Joback Method
dvisc	0.0050630	Pa×s	354.94	Joback Method
dvisc	0.0024676	Pa×s	384.55	Joback Method
dvisc	0.0013328	Pa×s	414.16	Joback Method
dvisc	0.0007816	Pa×s	443.76	Joback Method
dvisc	0.0004899	Pa×s	473.37	Joback Method
dvisc	0.0003245	Pa×s	502.98	Joback Method
dvisc	0.0002250	Pa×s	532.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.70	K	1.30	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=C75809&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

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