1,1,1-Tribromoethane

Inchi: InChI=1S/C2H3Br3/c1-2(3,4)5/h1H3
InchiKey: ZDUOUNIIAGIPSD-UHFFFAOYSA-N
Formula: C2H3Br3
SMILES: CC(Br)(Br)Br
Mol. weight [g/mol]: 266.76
CAS: 2311-14-0

Physical Properties

Property code	Value	Unit	Source
gf	11.76	kJ/mol	Joback Method
hf	-4.60	kJ/mol	NIST Webbook
hfus	9.38	kJ/mol	Joback Method
hvap	38.05	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.845		Crippen Method
mcvol	91.540	ml/mol	McGowan Method
pc	7133.40	kPa	Joback Method
tb	440.41	K	Joback Method
tc	689.34	K	Joback Method
tf	294.12	K	Joback Method
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.01	J/mol×K	440.41	Joback Method
cpg	121.95	J/mol×K	481.90	Joback Method
cpg	126.19	J/mol×K	523.39	Joback Method
cpg	129.83	J/mol×K	564.87	Joback Method
cpg	132.94	J/mol×K	606.36	Joback Method
cpg	135.59	J/mol×K	647.85	Joback Method
cpg	137.87	J/mol×K	689.34	Joback Method
dvisc	0.0032688	Pa×s	294.12	Joback Method
dvisc	0.0021590	Pa×s	318.50	Joback Method

dvisc	0.0015126	Pa×s	342.88	Joback Method
dvisc	0.0011111	Pa×s	367.26	Joback Method
dvisc	0.0008480	Pa×s	391.65	Joback Method
dvisc	0.0006681	Pa×s	416.03	Joback Method
dvisc	0.0005404	Pa×s	440.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39987e+01
Coeff. B	-3.69158e+03
Coeff. C	-6.51800e+01
Temperature range (K), min.	334.42
Temperature range (K), max.	490.12

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=C2311140&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume