Propane, 1,3-dibromo-2,2-dimethyl-

Other names: 1,3-Dibromo-2,2-dimethylpropane
Inchi: InChI=1S/C5H10Br2/c1-5(2,3-6)4-7/h3-4H2,1-2H3
InchiKey: UXAFLFGXSIWWMY-UHFFFAOYSA-N
Formula: C5H10Br2
SMILES: CC(C)(CBr)CBr
Mol. weight [g/mol]: 229.94
CAS: 5434-27-5

Physical Properties

Property code	Value	Unit	Source
gf	22.70	kJ/mol	Joback Method
hf	-102.62	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	38.30	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.802		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
tb	442.89	K	Joback Method
tc	661.07	K	Joback Method
tf	268.13	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.85	J/mol×K	442.89	Joback Method
cpg	208.11	J/mol×K	479.25	Joback Method
cpg	217.61	J/mol×K	515.62	Joback Method
cpg	226.38	J/mol×K	551.98	Joback Method
cpg	234.49	J/mol×K	588.34	Joback Method
cpg	242.00	J/mol×K	624.70	Joback Method
cpg	248.94	J/mol×K	661.07	Joback Method
dvisc	0.0043647	Pa×s	268.13	Joback Method

dvisc	0.0024400	Pa×s	297.26	Joback Method
dvisc	0.0015133	Pa×s	326.38	Joback Method
dvisc	0.0010149	Pa×s	355.51	Joback Method
dvisc	0.0007231	Pa×s	384.64	Joback Method
dvisc	0.0005404	Pa×s	413.76	Joback Method
dvisc	0.0004197	Pa×s	442.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48496e+01
Coeff. B	-4.03310e+03
Coeff. C	-6.79600e+01
Temperature range (K), min.	344.92
Temperature range (K), max.	490.80

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5434275&Units=SI

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

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

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