Propane, 1,3-dibromo-2,2-bis(bromomethyl)-

Other names:	1,3-Dibromo-2,2-bis(bromomethyl)propane
	2,2-Bis(bromomethyl)-1,3-dibromopropane
	NSC 8998
	Pentaerythritol tetrabromide
	Pentaerythrityl bromide
	Pentaerythrityl tetrabromide
	Tetra(bromomethyl)methane
	Tetrabromoneopentane
	Tetrakis(bromomethyl)methane
Inchi:	InChI=1S/C5H8Br4/c6-1-5(2-7,3-8)4-9/h1-4H2
InchiKey:	OYSVBCSOQFXYHK-UHFFFAOYSA-N
Formula:	C5H8Br4
SMILES:	BrCC(CBr)(CBr)CBr
Mol. weight [g/mol]:	387.73
CAS:	3229-00-3

Physical Properties

Property code	Value	Unit	Source
gf	51.34	kJ/mol	Joback Method
hf	-49.96	kJ/mol	Joback Method
hfus	22.43	kJ/mol	Joback Method
hvap	51.17	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.552		Crippen Method
mcvol	151.310	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
ss	297.12	J/mol×K	NIST Webbook
ss	291.12	J/mol×K	NIST Webbook
ss	291.12	J/mol×K	NIST Webbook
tb	578.70	K	NIST Webbook
tc	825.98	K	Joback Method
tf	387.73	K	Joback Method
tt	433.45 ± 0.05	K	NIST Webbook
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.41	J/mol×K	784.18	Joback Method
cpg	257.67	J/mol×K	575.21	Joback Method
cpg	265.61	J/mol×K	617.00	Joback Method
cpg	272.74	J/mol×K	658.80	Joback Method
cpg	279.17	J/mol×K	700.59	Joback Method
cpg	285.02	J/mol×K	742.39	Joback Method
cpg	295.44	J/mol×K	825.98	Joback Method
cps	213.80	J/mol×K	298.15	NIST Webbook
cps	218.57	J/mol×K	298.15	NIST Webbook
cps	213.80	J/mol×K	298.15	NIST Webbook
dvisc	0.0002958	Pa×s	575.21	Joback Method
dvisc	0.0018190	Pa×s	387.73	Joback Method
dvisc	0.0012004	Pa×s	418.98	Joback Method
dvisc	0.0008392	Pa×s	450.22	Joback Method
dvisc	0.0006146	Pa×s	481.47	Joback Method
dvisc	0.0004675	Pa×s	512.72	Joback Method
dvisc	0.0003670	Pa×s	543.96	Joback Method
hfust	27.97	kJ/mol	433.50	NIST Webbook
hfust	27.97	kJ/mol	433.45	NIST Webbook
hfust	27.97	kJ/mol	433.50	NIST Webbook
hsubt	84.00	kJ/mol	409.00	NIST Webbook
hvapt	61.00	kJ/mol	452.50	NIST Webbook
sfust	64.52	J/mol×K	433.45	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55318e+01
Coeff. B	-5.19682e+03
Coeff. C	-1.02015e+02
Temperature range (K), min.	436.15
Temperature range (K), max.	610.50

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3229003&Units=SI

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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