Pentaerythrityl tetraiodide

Other names:	2,2-Bis(iodomethyl)-1,3-diiodopropane
	Methane, tetrakis(iodomethyl)-
	Pentaerythritol tetraiodide
	Pentaerythrityl iodide
	Pentaerythryl tetraiodide
	Propane, 1,3-diiodo-2,2-bis(iodomethyl)-
	Propane, 2,2-bis(iodomethyl)-1,3-diiodo-
Inchi:	InChI=1S/C5H8I4/c6-1-5(2-7,3-8)4-9/h1-4H2
InchiKey:	HPMGSGCDKVCZHC-UHFFFAOYSA-N
Formula:	C5H8I4
SMILES:	ICC(CI)(CI)CI
Mol. weight [g/mol]:	575.73
CAS:	1522-88-9

Physical Properties

Property code	Value	Unit	Source
gf	226.54	kJ/mol	Joback Method
hf	152.20	kJ/mol	Joback Method
hfus	18.92	kJ/mol	Joback Method
hvap	62.92	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	3.713		Crippen Method
mcvol	184.590	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
ss	316.73	J/mol×K	NIST Webbook
ss	316.94	J/mol×K	NIST Webbook
tb	683.13	K	Joback Method
tc	1008.05	K	Joback Method
tf	380.77	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	294.28	J/mol×K	791.44	Joback Method
cpg	281.47	J/mol×K	683.13	Joback Method
cpg	288.25	J/mol×K	737.28	Joback Method
cpg	316.32	J/mol×K	1008.05	Joback Method
cpg	310.59	J/mol×K	953.89	Joback Method
cpg	305.19	J/mol×K	899.74	Joback Method
cpg	299.84	J/mol×K	845.59	Joback Method
cps	207.70	J/mol×K	298.15	NIST Webbook
cps	209.62	J/mol×K	298.15	NIST Webbook
cps	207.69	J/mol×K	298.15	NIST Webbook
dvisc	0.0001743	Pa×s	683.13	Joback Method
dvisc	0.0002318	Pa×s	632.74	Joback Method
dvisc	0.0003238	Pa×s	582.34	Joback Method
dvisc	0.0004818	Pa×s	531.95	Joback Method
dvisc	0.0007792	Pa×s	481.56	Joback Method
dvisc	0.0014099	Pa×s	431.16	Joback Method
dvisc	0.0029849	Pa×s	380.77	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38823e+01
Coeff. B	-5.25088e+03
Coeff. C	-1.29356e+02
Temperature range (K), min.	515.60
Temperature range (K), max.	742.00

Sources

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=C1522889&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

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
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume