

Octane, 1,8-diiodo-

Other names:	1,8-Diiodooctane Octamethylene diiodide
Inchi:	InChI=1S/C8H16I2/c9-7-5-3-1-2-4-6-8-10/h1-8H2
InchiKey:	KZDTZHQLABJVLE-UHFFFAOYSA-N
Formula:	C8H16I2
SMILES:	ICCCCCCCI
Mol. weight [g/mol]:	366.02
CAS:	24772-63-2

Physical Properties

Property code	Value	Unit	Source
gf	132.72	kJ/mol	Joback Method
hf	-54.71	kJ/mol	Joback Method
hfus	25.29	kJ/mol	Joback Method
hvap	52.15	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.197		Crippen Method
mvol	175.220	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
tb	568.72	K	Joback Method
tc	794.44	K	Joback Method
tf	296.04	K	Joback Method
vc	0.659	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.16	J/mol×K	568.72	Joback Method
cpg	354.83	J/mol×K	606.34	Joback Method
cpg	366.71	J/mol×K	643.96	Joback Method
cpg	377.87	J/mol×K	681.58	Joback Method
cpg	388.35	J/mol×K	719.20	Joback Method
cpg	398.21	J/mol×K	756.82	Joback Method
cpg	407.49	J/mol×K	794.44	Joback Method

dvisc	0.0047721	Paxs	296.04	Joback Method
dvisc	0.0021491	Paxs	341.49	Joback Method
dvisc	0.0011673	Paxs	386.93	Joback Method
dvisc	0.0007208	Paxs	432.38	Joback Method
dvisc	0.0004879	Paxs	477.83	Joback Method
dvisc	0.0003534	Paxs	523.27	Joback Method
dvisc	0.0002695	Paxs	568.72	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	441.20	K	0.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.60436e+01
Coeff. B	-5.50026e+03
Coeff. C	-1.03710e+02
Temperature range (K), min.	452.80
Temperature range (K), max.	616.21

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=C24772632&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/ci9903071
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
pvap:	Vapor 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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