

Oxonane

Other names:	Oxacyclononane Oxonin, octahydro-
Inchi:	InChI=1S/C8H16O/c1-2-4-6-8-9-7-5-3-1/h1-8H2
InchiKey:	YVQBOKCDPCUWSP-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	C1CCCCOCCC1
Mol. weight [g/mol]:	128.21
CAS:	6573-50-8

Physical Properties

Property code	Value	Unit	Source
gf	-73.78	kJ/mol	Joback Method
hf	-284.27	kJ/mol	Joback Method
hfus	8.92	kJ/mol	Joback Method
hvap	39.17	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.357		Crippen Method
mvol	118.590	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
rinpol	974.00		NIST Webbook
rinpol	974.00		NIST Webbook
tb	446.42	K	Joback Method
tc	673.75	K	Joback Method
tf	207.55	K	Joback Method
vc	0.414	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.57	J/mol×K	446.42	Joback Method
cpg	262.59	J/mol×K	484.31	Joback Method
cpg	281.58	J/mol×K	522.20	Joback Method
cpg	299.54	J/mol×K	560.08	Joback Method
cpg	316.47	J/mol×K	597.97	Joback Method

cpg	332.40	J/molxK	635.86	Joback Method
cpg	347.32	J/molxK	673.75	Joback Method
dvisc	0.0749594	Paxs	207.55	Joback Method
dvisc	0.0125704	Paxs	247.36	Joback Method
dvisc	0.0034585	Paxs	287.17	Joback Method
dvisc	0.0013029	Paxs	326.99	Joback Method
dvisc	0.0006067	Paxs	366.80	Joback Method
dvisc	0.0003281	Paxs	406.61	Joback Method
dvisc	0.0001980	Paxs	446.42	Joback Method

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=C6573508&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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