

Benzofuran, octahydro-, cis-

Inchi:	InChI=1S/C8H14O/c1-2-4-8-7(3-1)5-6-9-8/h7-8H,1-6H2/t7-,8-/m0/s1
InchiKey:	DNZWAKVIOXCEHH-YUMQZZPRSA-N
Formula:	C8H14O
SMILES:	C1CCC2OCCC2C1
Mol. weight [g/mol]:	126.20
CAS:	10198-29-5

Physical Properties

Property code	Value	Unit	Source
gf	15.56	kJ/mol	Joback Method
hf	-213.33	kJ/mol	Joback Method
hfus	14.42	kJ/mol	Joback Method
hvap	38.25	kJ/mol	Joback Method
ie	9.00	eV	NIST Webbook
ie	9.24 ± 0.04	eV	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.965		Crippen Method
mcvol	107.730	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	435.68	K	Joback Method
tc	654.15	K	Joback Method
tf	231.81	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.10	J/molxK	435.68	Joback Method
cpg	312.50	J/molxK	617.73	Joback Method
cpg	298.13	J/molxK	581.32	Joback Method
cpg	282.76	J/molxK	544.91	Joback Method
cpg	266.33	J/molxK	508.50	Joback Method
cpg	248.80	J/molxK	472.09	Joback Method
cpg	325.93	J/molxK	654.15	Joback Method

dvisc	0.0005316	Paxs	435.68	Joback Method
dvisc	0.0006330	Paxs	401.70	Joback Method
dvisc	0.0007784	Paxs	367.72	Joback Method
dvisc	0.0009983	Paxs	333.75	Joback Method
dvisc	0.0013548	Paxs	299.77	Joback Method
dvisc	0.0019879	Paxs	265.79	Joback Method
dvisc	0.0032638	Paxs	231.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10198295&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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