

trans-7-Oxabicyclo[4.3.0]nonane

Other names:	Benzofuran, octahydro-, trans-
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-JGVFFNPUSA-N
Formula:	C8H14O
SMILES:	C1CCC2OCCC2C1
Mol. weight [g/mol]:	126.20
CAS:	27345-70-6

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/mol×K	435.68	Joback Method
cpg	248.80	J/mol×K	472.09	Joback Method
cpg	266.33	J/mol×K	508.50	Joback Method
cpg	282.76	J/mol×K	544.91	Joback Method
cpg	298.13	J/mol×K	581.32	Joback Method
cpg	312.50	J/mol×K	617.73	Joback Method

cpg	325.93	J/mol×K	654.15	Joback Method
dvisc	0.0032638	Pa×s	231.81	Joback Method
dvisc	0.0019879	Pa×s	265.79	Joback Method
dvisc	0.0013548	Pa×s	299.77	Joback Method
dvisc	0.0009983	Pa×s	333.75	Joback Method
dvisc	0.0007784	Pa×s	367.72	Joback Method
dvisc	0.0006330	Pa×s	401.70	Joback Method
dvisc	0.0005316	Pa×s	435.68	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=C27345706&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
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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