

2,3-DIOXABICYCLO[2.2.2]OCT-7-ENE

Other names:	2,3-Dioxabicyclo[2.2.2]oct-7-ene
Inchi:	InChI=1S/C6H8O2/c1-2-6-4-3-5(1)7-8-6/h1-2,5-6H,3-4H2
InchiKey:	AHUADBUKFJZUTM-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	C1=CC2CCC1OO2
Mol. weight [g/mol]:	112.13

Physical Properties

Property code	Value	Unit	Source
hfus	20.55	kJ/mol	Joback Method
ie	8.76	eV	NIST Webbook
logp	1.035		Crippen Method
mcvol	81.120	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.83	J/mol×K	411.76	Joback Method
cpg	179.32	J/mol×K	447.89	Joback Method
cpg	191.87	J/mol×K	484.01	Joback Method
cpg	203.53	J/mol×K	520.14	Joback Method
cpg	214.36	J/mol×K	556.27	Joback Method
cpg	224.40	J/mol×K	592.40	Joback Method
cpg	233.71	J/mol×K	628.52	Joback Method
dvisc	0.0018938	Pa×s	240.12	Joback Method
dvisc	0.0014333	Pa×s	268.73	Joback Method
dvisc	0.0011445	Pa×s	297.33	Joback Method
dvisc	0.0009507	Pa×s	325.94	Joback Method
dvisc	0.0008138	Pa×s	354.55	Joback Method
dvisc	0.0007129	Pa×s	383.15	Joback Method
dvisc	0.0006361	Pa×s	411.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6671701&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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