

2,3-Dioxabicyclo[2.2.2]oct-5-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
CAS:	6671-70-1

Physical Properties

Property code	Value	Unit	Source
gf	-45.34	kJ/mol	Joback Method
hf	-240.11	kJ/mol	Joback Method
hfus	20.55	kJ/mol	Joback Method
hvap	38.43	kJ/mol	Joback Method
ie	8.76	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.035		Crippen Method
mcvol	81.120	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	411.76	K	Joback Method
tc	628.52	K	Joback Method
tf	240.12	K	Joback Method
vc	0.297	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.83	J/molxK	411.76	Joback Method
cpg	179.32	J/molxK	447.89	Joback Method
cpg	191.87	J/molxK	484.01	Joback Method
cpg	203.53	J/molxK	520.14	Joback Method
cpg	214.36	J/molxK	556.27	Joback Method
cpg	224.40	J/molxK	592.40	Joback Method
cpg	233.71	J/molxK	628.52	Joback Method

dvisc	0.0018938	Paxs	240.12	Joback Method
dvisc	0.0014333	Paxs	268.73	Joback Method
dvisc	0.0011445	Paxs	297.33	Joback Method
dvisc	0.0009507	Paxs	325.94	Joback Method
dvisc	0.0008138	Paxs	354.55	Joback Method
dvisc	0.0007129	Paxs	383.15	Joback Method
dvisc	0.0006361	Paxs	411.76	Joback Method

Sources

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

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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