

2,3-Dioxabicyclo[2.2.2]octane

Inchi:	InChI=1S/C6H10O2/c1-2-6-4-3-5(1)7-8-6/h5-6H,1-4H2
InchiKey:	BFPOIBUGVNVNKH-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	C1CC2CCC1OO2
Mol. weight [g/mol]:	114.14
CAS:	280-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-75.30	kJ/mol	Joback Method
hf	-297.89	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	38.14	kJ/mol	Joback Method
ie	8.83	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
log10ws	-1.51		Crippen Method
logp	1.259		Crippen Method
mcvol	85.420	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
tb	412.60	K	Joback Method
tc	627.05	K	Joback Method
tf	239.36	K	Joback Method
vc	0.311	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.02	J/molxK	412.60	Joback Method
cpg	193.88	J/molxK	448.34	Joback Method
cpg	207.76	J/molxK	484.08	Joback Method
cpg	220.73	J/molxK	519.82	Joback Method
cpg	232.84	J/molxK	555.57	Joback Method
cpg	244.12	J/molxK	591.31	Joback Method
cpg	254.64	J/molxK	627.05	Joback Method

dvisc	0.0023936	Paxs	239.36	Joback Method
dvisc	0.0017282	Paxs	268.23	Joback Method
dvisc	0.0013294	Paxs	297.11	Joback Method
dvisc	0.0010712	Paxs	325.98	Joback Method
dvisc	0.0008941	Paxs	354.85	Joback Method
dvisc	0.0007668	Paxs	383.73	Joback Method
dvisc	0.0006719	Paxs	412.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C280535&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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