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: BFPOIBUGVNVNKU-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/mol×K	412.60	Joback Method
cpg	193.88	J/mol×K	448.34	Joback Method
cpg	207.76	J/mol×K	484.08	Joback Method
cpg	220.73	J/mol×K	519.82	Joback Method
cpg	232.84	J/mol×K	555.57	Joback Method
cpg	244.12	J/mol×K	591.31	Joback Method
cpg	254.64	J/mol×K	627.05	Joback Method

dvisc	0.0023936	Pa×s	239.36	Joback Method
dvisc	0.0017282	Pa×s	268.23	Joback Method
dvisc	0.0013294	Pa×s	297.11	Joback Method
dvisc	0.0010712	Pa×s	325.98	Joback Method
dvisc	0.0008941	Pa×s	354.85	Joback Method
dvisc	0.0007668	Pa×s	383.73	Joback Method
dvisc	0.0006719	Pa×s	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/ci990307l
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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