2,3-Dioxabicyclo[2.2.1]heptane

Inchi: InChI=1S/C5H8O2/c1-2-5-3-4(1)6-7-5/h4-5H,1-3H2
InchiKey: RNFXAEBUWFIOQW-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: C1CC2CC1OO2
Mol. weight [g/mol]: 100.12
CAS: 279-35-6

Physical Properties

Property code	Value	Unit	Source
gf	-71.62	kJ/mol	Joback Method
hf	-271.09	kJ/mol	Joback Method
hfus	18.83	kJ/mol	Joback Method
hvap	35.74	kJ/mol	Joback Method
ie	8.99	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
log10ws	-1.09		Crippen Method
logp	0.869		Crippen Method
mcvol	71.330	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	385.45	K	Joback Method
tc	593.06	K	Joback Method
tf	231.61	K	Joback Method
vc	0.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.40	J/mol×K	385.45	Joback Method
cpg	155.11	J/mol×K	420.05	Joback Method
cpg	166.95	J/mol×K	454.65	Joback Method
cpg	177.97	J/mol×K	489.26	Joback Method
cpg	188.22	J/mol×K	523.86	Joback Method
cpg	197.75	J/mol×K	558.46	Joback Method

cpg	206.61	J/mol×K	593.06	Joback Method
dvisc	0.0013677	Pa×s	231.61	Joback Method
dvisc	0.0011432	Pa×s	257.25	Joback Method
dvisc	0.0009871	Pa×s	282.89	Joback Method
dvisc	0.0008734	Pa×s	308.53	Joback Method
dvisc	0.0007874	Pa×s	334.17	Joback Method
dvisc	0.0007205	Pa×s	359.81	Joback Method
dvisc	0.0006670	Pa×s	385.45	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C279356&Units=SI

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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