2,5-Dioxanonane

Inchi:	InChI=1S/C7H16O2/c1-3-4-5-9-7-6-8-2/h3-7H2,1-2H3
InchiKey:	XDFQEFFBRPGSMC-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CCCCOCCOC
Mol. weight [g/mol]:	132.20
CAS:	500005-29-8

Physical Properties

Property code	Value	Unit	Source
gf	-201.94	kJ/mol	Joback Method
hf	-452.25	kJ/mol	Joback Method
hfus	16.26	kJ/mol	Joback Method
hvap	36.00	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	1.450		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	404.40	K	Joback Method
tc	569.26	K	Joback Method
tf	213.11	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.33	J/mol×K	404.40	Joback Method
cpg	305.65	J/mol×K	569.26	Joback Method
cpg	295.82	J/mol×K	541.78	Joback Method
cpg	285.69	J/mol×K	514.30	Joback Method
cpg	275.28	J/mol×K	486.83	Joback Method
cpg	264.58	J/mol×K	459.35	Joback Method
cpg	253.59	J/mol×K	431.88	Joback Method
cpl	282.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0001992	Pa×s	404.40	Joback Method

dvisc	0.0002575	Pa×s	372.52	Joback Method
dvisc	0.0003493	Pa×s	340.64	Joback Method
dvisc	0.0005047	Pa×s	308.75	Joback Method
dvisc	0.0007936	Pa×s	276.87	Joback Method
dvisc	0.0014040	Pa×s	244.99	Joback Method
dvisc	0.0029460	Pa×s	213.11	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=C500005298&Units=SI

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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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