

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/molxK	404.40	Joback Method
cpg	253.59	J/molxK	431.88	Joback Method
cpg	264.58	J/molxK	459.35	Joback Method
cpg	275.28	J/molxK	486.83	Joback Method
cpg	285.69	J/molxK	514.30	Joback Method
cpg	295.82	J/molxK	541.78	Joback Method
cpg	305.65	J/molxK	569.26	Joback Method
cpl	282.00	J/molxK	298.15	NIST Webbook
dvisc	0.0029460	Paxs	213.11	Joback Method

dvisc	0.0014040	Paxs	244.99	Joback Method
dvisc	0.0007936	Paxs	276.87	Joback Method
dvisc	0.0005047	Paxs	308.75	Joback Method
dvisc	0.0003493	Paxs	340.64	Joback Method
dvisc	0.0002575	Paxs	372.52	Joback Method
dvisc	0.0001992	Paxs	404.40	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
cp_l:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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