

4-Piperidinone ethyl ketal

Other names:	Piperidone-4-ethyleneketal 4-Piperidone ethylene ketal 1,4-Dioxa-8-azaspiro[4,5]decane 1,4-dioxa-8-azaspiro[4.5]decane
Inchi:	InChI=1S/C7H13NO2/c1-3-8-4-2-7(1)9-5-6-10-7/h8H,1-6H2
InchiKey:	KPKNTUUIEVXMOH-UHFFFAOYSA-N
Formula:	C7H13NO2
SMILES:	C1CC2(CCN1)OCCO2
Mol. weight [g/mol]:	143.18
CAS:	177-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-1.15	kJ/mol	Joback Method
hf	-257.46	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	46.63	kJ/mol	Joback Method
log10ws	-0.51		Crippen Method
logp	0.113		Crippen Method
mcvol	109.490	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
tb	497.48	K	Joback Method
tc	744.68	K	Joback Method
tf	376.76	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.20	J/molxK	497.48	Joback Method
cpg	278.66	J/molxK	538.68	Joback Method
cpg	294.68	J/molxK	579.88	Joback Method
cpg	309.45	J/molxK	621.08	Joback Method
cpg	323.15	J/molxK	662.28	Joback Method

cpg	335.96	J/mol×K	703.48	Joback Method
cpg	348.05	J/mol×K	744.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	3.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C177117&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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