2H-Azepine, 3,4,5,6-tetrahydro-7-methoxy-

Other names:	7-Methoxy-3,4,5,6-tetrahydro-2H-azepine
	1-Aza-2-methoxy-1-cycloheptane
	O-Methylcaprolactim
	Caprolactim methyl ether
	Caprolactim-O-methyl ether
	O-Methyl-«epsilon»-caprolactim
	O-Methylhexanolactim
	2-Methoxy-1-azacycloheptene
	3,4,5,6-Tetrahydro-7-methoxy-2H-azepine
	«epsilon»-Caprolactim methyl ether
	2-Methoxy-4,5,6,7-tetrahydro-3H-azepine
	NSC 31263
	NSC 523095
	methyl 3,4,5,6-tetrahydro-7H-azepin-2-yl ether
Inchi:	InChI=1S/C7H13NO/c1-9-7-5-3-2-4-6-8-7/h2-6H2,1H3
InchiKey:	DNXIQMQGKSQHPC-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	COC1=NCCCCC1
Mol. weight [g/mol]:	127.18
CAS:	2525-16-8

Physical Properties

Property code	Value	Unit	Source
gf	60.23	kJ/mol	Joback Method
hf	-134.25	kJ/mol	Joback Method
hfus	9.71	kJ/mol	Joback Method
hvap	41.66	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.605		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	468.31	K	Joback Method
tc	695.53	K	Joback Method
tf	283.80	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.16	J/mol×K	468.31	Joback Method
cpg	256.05	J/mol×K	506.18	Joback Method
cpg	272.17	J/mol×K	544.05	Joback Method
cpg	287.51	J/mol×K	581.92	Joback Method
cpg	302.05	J/mol×K	619.79	Joback Method
cpg	315.77	J/mol×K	657.66	Joback Method
cpg	328.65	J/mol×K	695.53	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	325.70	K	2.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2525168&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

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