o-Methylvalerolactim

Inchi: InChI=1S/C6H11NO/c1-8-6-4-2-3-5-7-6/h2-5H2,1H3
InchiKey: YNTUHDRALXNDEQ-UHFFFAOYSA-N
Formula: C6H11NO
SMILES: COC1=NCCCC1
Mol. weight [g/mol]: 113.16
CAS: 5693-62-9

Physical Properties

Property code	Value	Unit	Source
gf	63.91	kJ/mol	Joback Method
hf	-107.45	kJ/mol	Joback Method
hfus	9.22	kJ/mol	Joback Method
hvap	39.26	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	1.215		Crippen Method
mcvol	96.090	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
tb	441.16	K	Joback Method
tc	662.76	K	Joback Method
tf	276.05	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.05	J/mol×K	441.16	Joback Method
cpg	212.60	J/mol×K	478.09	Joback Method
cpg	226.52	J/mol×K	515.03	Joback Method
cpg	239.80	J/mol×K	551.96	Joback Method
cpg	252.44	J/mol×K	588.89	Joback Method
cpg	264.42	J/mol×K	625.83	Joback Method
cpg	275.74	J/mol×K	662.76	Joback Method
hvapt	42.80	kJ/mol	315.00	NIST Webbook
hvapt	41.00 ± 3.10	kJ/mol	403.00	NIST Webbook

Sources

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=C5693629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
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