3,4-Dihydro-6-methyl-2H-pyran-2-one

Other names: 6-Methyl-3,4-dihydropyran-2-one
Inchi: InChI=1S/C6H8O2/c1-5-3-2-4-6(7)8-5/h3H,2,4H2,1H3
InchiKey: DOSOPEZOHKMQPJ-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: CC1=CCCC(=O)O1
Mol. weight [g/mol]: 112.13
CAS: 3740-59-8

Physical Properties

Property code	Value	Unit	Source
gf	-156.58	kJ/mol	Joback Method
hf	-315.90	kJ/mol	Joback Method
hfus	10.38	kJ/mol	Joback Method
hvap	39.40	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	1.227		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
ripol	1585.00		NIST Webbook
ripol	1585.00		NIST Webbook
tb	459.81	K	Joback Method
tc	689.89	K	Joback Method
tf	277.07	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.28	J/mol×K	459.81	Joback Method
cpg	188.09	J/mol×K	498.16	Joback Method
cpg	199.41	J/mol×K	536.50	Joback Method
cpg	210.21	J/mol×K	574.85	Joback Method
cpg	220.50	J/mol×K	613.20	Joback Method
cpg	230.25	J/mol×K	651.55	Joback Method

cpg	239.44	J/mol×K	689.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.70	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3740598&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume