Furan-2-carboxaldehyde, 3-methyl

Inchi: InChI=1S/C7H8O/c1-6-3-2-4-7(6)5-8/h2-3,5H,4H2,1H3
InchiKey: SOVBMQDVRPCJDH-UHFFFAOYSA-N
Formula: C7H8O
SMILES: CC1=C(C=O)CC=C1
Mol. weight [g/mol]: 108.14

Physical Properties

Property code	Value	Unit	Source
gf	-6.54	kJ/mol	Joback Method
hf	-99.95	kJ/mol	Joback Method
hfus	10.71	kJ/mol	Joback Method
hvap	40.37	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.462		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
rinpol	938.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	934.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1562.00		NIST Webbook
tb	436.45	K	Joback Method
tc	645.82	K	Joback Method
tf	252.35	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.56	J/mol×K	436.45	Joback Method
cpg	181.73	J/mol×K	471.35	Joback Method
cpg	191.31	J/mol×K	506.24	Joback Method
cpg	200.34	J/mol×K	541.14	Joback Method

cpg	208.84	J/mol×K	576.03	Joback Method
cpg	216.84	J/mol×K	610.93	Joback Method
cpg	224.36	J/mol×K	645.82	Joback Method
dvisc	0.0019115	Pa×s	252.35	Joback Method
dvisc	0.0012298	Pa×s	283.03	Joback Method
dvisc	0.0008624	Pa×s	313.72	Joback Method
dvisc	0.0006443	Pa×s	344.40	Joback Method
dvisc	0.0005049	Pa×s	375.08	Joback Method
dvisc	0.0004105	Pa×s	405.77	Joback Method
dvisc	0.0003436	Pa×s	436.45	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R68277&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas 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: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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