Furan-2-carboxaldehyde, 3,5-dimethyl

Inchi: InChI=1S/C8H10O/c1-6-3-7(2)8(4-6)5-9/h3,5H,4H2,1-2H3
InchiKey: MWKCFGKWTQJWNR-UHFFFAOYSA-N
Formula: C8H10O
SMILES: CC1=CC(C)=C(C=O)C1
Mol. weight [g/mol]: 122.16

Physical Properties

Property code	Value	Unit	Source
gf	-7.75	kJ/mol	Joback Method
hf	-132.06	kJ/mol	Joback Method
hfus	12.91	kJ/mol	Joback Method
hvap	43.26	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.852		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	1021.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1019.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1664.00		NIST Webbook
tb	464.31	K	Joback Method
tc	672.36	K	Joback Method
tf	276.14	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.03	J/mol×K	464.31	Joback Method
cpg	222.01	J/mol×K	498.98	Joback Method
cpg	232.42	J/mol×K	533.66	Joback Method
cpg	242.29	J/mol×K	568.33	Joback Method

cpg	251.63	J/mol×K	603.01	Joback Method
cpg	260.46	J/mol×K	637.68	Joback Method
cpg	268.81	J/mol×K	672.36	Joback Method
dvisc	0.0015995	Pa×s	276.14	Joback Method
dvisc	0.0010775	Pa×s	307.50	Joback Method
dvisc	0.0007809	Pa×s	338.86	Joback Method
dvisc	0.0005977	Pa×s	370.22	Joback Method
dvisc	0.0004770	Pa×s	401.59	Joback Method
dvisc	0.0003933	Pa×s	432.95	Joback Method
dvisc	0.0003328	Pa×s	464.31	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R68263&Units=SI

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