2,5-Furnadione, 3-(1-methylethyl)-

Inchi: InChI=1S/C7H8O3/c1-4(2)5-3-6(8)10-7(5)9/h3-4H,1-2H3
InchiKey: QSWLSAYLEATCSH-UHFFFAOYSA-N
Formula: C7H8O3
SMILES: CC(C)C1=CC(=O)OC1=O
Mol. weight [g/mol]: 140.14
CAS: 64198-15-8

Physical Properties

Property code	Value	Unit	Source
gf	-261.09	kJ/mol	Joback Method
hf	-473.36	kJ/mol	Joback Method
hfus	11.06	kJ/mol	Joback Method
hvap	45.31	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.652		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
tb	545.80	K	Joback Method
tc	785.16	K	Joback Method
tf	345.08	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.54	J/mol×K	545.80	Joback Method
cpg	251.91	J/mol×K	585.69	Joback Method
cpg	263.76	J/mol×K	625.59	Joback Method
cpg	275.03	J/mol×K	665.48	Joback Method
cpg	285.69	J/mol×K	705.37	Joback Method
cpg	295.69	J/mol×K	745.27	Joback Method
cpg	304.98	J/mol×K	785.16	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=C64198158&Units=SI

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume