3-Ethyl-4-methyl-2,5-furandione

Other names: 3-Ethyl-4-methyl-2,5-furanedione
Inchi: InChI=1S/C7H8O3/c1-3-5-4(2)6(8)10-7(5)9/h3H2,1-2H3
InchiKey: ZVUUAOZFEUKPLC-UHFFFAOYSA-N
Formula: C7H8O3
SMILES: CCC1=C(C)C(=O)OC1=O
Mol. weight [g/mol]: 140.14
CAS: 3552-33-8

Physical Properties

Property code	Value	Unit	Source
gf	-268.28	kJ/mol	Joback Method
hf	-479.55	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	46.36	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	0.796		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
ripol	1777.00		NIST Webbook
ripol	1777.00		NIST Webbook
ripol	1777.00		NIST Webbook
tb	551.22	K	Joback Method
tc	786.26	K	Joback Method
tf	372.60	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.44	J/mol×K	551.22	Joback Method
cpg	250.17	J/mol×K	590.39	Joback Method
cpg	261.47	J/mol×K	629.57	Joback Method
cpg	272.28	J/mol×K	668.74	Joback Method
cpg	282.57	J/mol×K	707.91	Joback Method

cpg	292.28	J/mol×K	747.08	Joback Method
cpg	301.35	J/mol×K	786.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3552338&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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