3-Ethyl-4-methylpyrollidindione

Inchi: InChI=1S/C7H11NO2/c1-3-5-4(2)6(9)8-7(5)10/h4-5H,3H2,1-2H3,(H,8,9,10)
InchiKey: NEXJJNOSOSCCPR-UHFFFAOYSA-N
Formula: C7H11NO2
SMILES: CCC1C(=O)NC(=O)C1C
Mol. weight [g/mol]: 141.17

Physical Properties

Property code	Value	Unit	Source
gf	-120.57	kJ/mol	Joback Method
hf	-385.26	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	46.38	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.305		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	1307.00		NIST Webbook
tb	554.36	K	Joback Method
tc	791.50	K	Joback Method
tf	416.78	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.69	J/mol×K	554.36	Joback Method
cpg	289.01	J/mol×K	593.88	Joback Method
cpg	303.74	J/mol×K	633.41	Joback Method
cpg	317.79	J/mol×K	672.93	Joback Method
cpg	331.11	J/mol×K	712.46	Joback Method
cpg	343.63	J/mol×K	751.98	Joback Method
cpg	355.29	J/mol×K	791.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R416298&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume