trans-Dihydro-3,4-diethyl-2,5-furandione

Inchi: InChI=1S/C8H12O3/c1-3-5-6(4-2)8(10)11-7(5)9/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1
InchiKey: WRAJQNMZXMXFND-WDSKDSINSA-N
Formula: C8H12O3
SMILES: CCC1C(=O)OC(=O)C1CC
Mol. weight [g/mol]: 156.18
CAS: 35046-86-7

Physical Properties

Property code	Value	Unit	Source
chl	-4163.00 ± 2.10	kJ/mol	NIST Webbook
gf	-285.98	kJ/mol	Joback Method
hf	-575.71	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	46.35	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.122		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
tb	555.64	K	Joback Method
tc	781.65	K	Joback Method
tf	349.59	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.23	J/mol×K	555.64	Joback Method
cpg	322.77	J/mol×K	593.31	Joback Method
cpg	337.66	J/mol×K	630.98	Joback Method
cpg	351.86	J/mol×K	668.64	Joback Method
cpg	365.31	J/mol×K	706.31	Joback Method
cpg	377.98	J/mol×K	743.98	Joback Method
cpg	389.82	J/mol×K	781.65	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=C35046867&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
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