2-methoxy-3,5,5-trimethylcyclohex-2-ene-1,4-dion

Inchi: InChI=1S/C10H14O3/c1-6-8(13-4)7(11)5-10(2,3)9(6)12/h5H2,1-4H3
InchiKey: ATEVRAIEOLFIJD-UHFFFAOYSA-N
Formula: C10H14O3
SMILES: COC1=C(C)C(=O)C(C)(C)CC1=O
Mol. weight [g/mol]: 182.22
CAS: 41654-27-7

Physical Properties

Property code	Value	Unit	Source
gf	-287.20	kJ/mol	Joback Method
hf	-552.95	kJ/mol	Joback Method
hfus	7.85	kJ/mol	Joback Method
hvap	49.65	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.475		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
tb	615.17	K	Joback Method
tc	853.35	K	Joback Method
tf	418.21	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.71	J/mol×K	615.17	Joback Method
cpg	390.90	J/mol×K	654.87	Joback Method
cpg	406.43	J/mol×K	694.56	Joback Method
cpg	421.31	J/mol×K	734.26	Joback Method
cpg	435.59	J/mol×K	773.95	Joback Method
cpg	449.30	J/mol×K	813.65	Joback Method
cpg	462.48	J/mol×K	853.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41654277&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume