3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene-2,5-dione

Inchi: InChI=1S/C10H12O2/c1-5-4-6(11)7-8(9(5)12)10(7,2)3/h4,7-8H,1-3H3
InchiKey: BBRJZZUFDYMNIY-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC1=CC(=O)C2C(C1=O)C2(C)C
Mol. weight [g/mol]: 164.20
CAS: 6617-34-1

Physical Properties

Property code	Value	Unit	Source
gf	-95.33	kJ/mol	Joback Method
hf	-344.48	kJ/mol	Joback Method
hfus	10.45	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.357		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1324.10		NIST Webbook
tb	581.30	K	Joback Method
tc	822.92	K	Joback Method
tf	404.20	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.42	J/mol×K	581.30	Joback Method
cpg	351.28	J/mol×K	621.57	Joback Method
cpg	366.28	J/mol×K	661.84	Joback Method
cpg	380.54	J/mol×K	702.11	Joback Method
cpg	394.18	J/mol×K	742.38	Joback Method
cpg	407.31	J/mol×K	782.65	Joback Method
cpg	420.04	J/mol×K	822.92	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=C6617341&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume