Bicyclo[2.2.1]heptane-2,3-dione, 1,7,7-trimethyl-, (1S)-

Other names:	(+)-camphorquinone
	(1S)-(+)-camphorquinone
	(1S)-1,7,7-trimethylbicyclo[2.2.1]heptane-2,3-dione
	2,3-bornanedione, (1S,4R)-(+)-
	D(+)-camphorquinone
	Dl-camphorquinone
	d-camphorquinone
Inchi:	InChI=1S/C10H14O2/c1-9(2)6-4-5-10(9,3)8(12)7(6)11/h6H,4-5H2,1-3H3/t6-,10+/m0/s1
InchiKey:	VNQXSTWCDUXYEZ-QUBYGPBYSA-N
Formula:	C10H14O2
SMILES:	CC12CCC(C(=O)C1=O)C2(C)C
Mol. weight [g/mol]:	166.22
CAS:	2767-84-2

Physical Properties

Property code	Value	Unit	Source
gf	-121.15	kJ/mol	Joback Method
hf	-375.55	kJ/mol	Joback Method
hfus	3.32	kJ/mol	Joback Method
hvap	43.73	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.581		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
tb	577.40	K	Joback Method
tc	825.69	K	Joback Method
tf	414.82	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.37	J/mol×K	784.31	Joback Method
cpg	354.19	J/mol×K	577.40	Joback Method

cpg	371.27	J/mol×K	618.78	Joback Method
cpg	387.37	J/mol×K	660.16	Joback Method
cpg	402.74	J/mol×K	701.54	Joback Method
cpg	417.65	J/mol×K	742.93	Joback Method
cpg	447.14	J/mol×K	825.69	Joback Method
hfust	6.07	kJ/mol	473.20	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of ethanol solution of chiral camphors and its derivatives:	https://www.doi.org/10.1016/j.jct.2009.05.005
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=C2767842&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
hfust:	Enthalpy of fusion at a given temperature
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

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