Bicyclo[2.2.1]heptane-2,5-dione, 1,7,7-trimethyl-

Other names: 2,5-Bornanedione
Inchi: InChI=1S/C10H14O2/c1-9(2)6-4-8(12)10(9,3)5-7(6)11/h6H,4-5H2,1-3H3
InchiKey: UDIUFGIXIGLRSM-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC12CC(=O)C(CC1=O)C2(C)C
Mol. weight [g/mol]: 166.22
CAS: 4230-32-4

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
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
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	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	432.37	J/mol×K	784.31	Joback Method

cpg	447.14	J/mol×K	825.69	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=C4230324&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