Tricyclo[4.2.1.02,5]non-7-ene-3,4-dione, (1«alpha»,2«beta»,5«beta»,6«alpha»)-

Inchi: InChI=1S/C9H8O2/c10-8-6-4-1-2-5(3-4)7(6)9(8)11/h1-2,4-7H,3H2/t4?,5?,6-,7+

InchiKey: RFKYFDOSOGLBRF-CYDAGYADSA-N

Formula: C9H8O2

SMILES: O=C1C(=O)C2C3C=CC(C3)C12

Mol. weight [g/mol]: 148.16

CAS: 67792-55-6

Physical Properties

Property code	Value	Unit	Source
gf	-15.78	kJ/mol	Joback Method
hf	-248.65	kJ/mol	Joback Method
hfus	14.78	kJ/mol	Joback Method
hvap	43.84	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
log10ws	-0.72		Crippen Method
logp	0.576		Crippen Method
mcvol	103.930	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
tb	555.67	K	Joback Method
tc	800.73	K	Joback Method
tf	377.97	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.03	J/mol×K	555.67	Joback Method
cpg	290.49	J/mol×K	596.51	Joback Method
cpg	304.91	J/mol×K	637.36	Joback Method
cpg	318.34	J/mol×K	678.20	Joback Method
cpg	330.85	J/mol×K	719.04	Joback Method
cpg	342.48	J/mol×K	759.89	Joback Method
cpg	353.31	J/mol×K	800.73	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=C67792556&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
ie:	Ionization energy
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