2-Allyl-2-methyl-1,3-cyclopentanedione

Inchi: InChI=1S/C9H12O2/c1-3-6-9(2)7(10)4-5-8(9)11/h3H,1,4-6H2,2H3
InchiKey: MCOMBKZMVPQQKK-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: C=CCC1(C)C(=O)CCC1=O
Mol. weight [g/mol]: 152.19
CAS: 26828-48-8

Physical Properties

Property code	Value	Unit	Source
gf	-101.38	kJ/mol	Joback Method
hf	-303.34	kJ/mol	Joback Method
hfus	4.44	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.501		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	553.16	K	Joback Method
tc	792.19	K	Joback Method
tf	360.67	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.11	J/mol×K	553.16	Joback Method
cpg	317.65	J/mol×K	593.00	Joback Method
cpg	332.37	J/mol×K	632.84	Joback Method
cpg	346.34	J/mol×K	672.68	Joback Method
cpg	359.66	J/mol×K	712.52	Joback Method
cpg	372.40	J/mol×K	752.35	Joback Method
cpg	384.65	J/mol×K	792.19	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	334.70	K	0.10	NIST Webbook

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=C26828488&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume