1-PHENYL-1,4-PENTANEDIONE

Other names: 1-Phenyl-1,4-pentanedione
Inchi: InChI=1S/C11H12O2/c1-9(12)7-8-11(13)10-5-3-2-4-6-10/h2-6H,7-8H2,1H3
InchiKey: RBLXWIPBPPVLPU-UHFFFAOYSA-N
Formula: C11H12O2
SMILES: CC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 176.22

Physical Properties

Property code	Value	Unit	Source
af	0.5346		Cheméo Relay (1.0)
gf	-103.69	kJ/mol	Joback Method
hf	-262.50	kJ/mol	Cheméo Relay (1.0)
hfus	21.49	kJ/mol	Joback Method
hvap	71.84	kJ/mol	Cheméo Relay (1.0)
ie	9.07	eV	Cheméo Relay (1.0)
log10ws	-1.57		Cheméo Relay (1.0)
logp	2.239		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
tb	552.75	K	Cheméo Relay (1.0)
tc	760.91	K	Cheméo Relay (1.0)
tf	329.14	K	Cheméo Relay (1.0)
vc	0.523	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.46	J/mol×K	585.50	Joback Method
cpg	352.88	J/mol×K	622.10	Joback Method
cpg	365.41	J/mol×K	658.70	Joback Method
cpg	377.09	J/mol×K	695.31	Joback Method
cpg	387.96	J/mol×K	731.91	Joback Method
cpg	398.06	J/mol×K	768.51	Joback Method
cpg	407.41	J/mol×K	805.11	Joback Method

dvisc	0.0026331	Pa×s	340.01	Joback Method
dvisc	0.0014576	Pa×s	380.93	Joback Method
dvisc	0.0009050	Pa×s	421.84	Joback Method
dvisc	0.0006113	Pa×s	462.75	Joback Method
dvisc	0.0004401	Pa×s	503.67	Joback Method
dvisc	0.0003329	Pa×s	544.59	Joback Method
dvisc	0.0002618	Pa×s	585.50	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C583051&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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