1,3-Diphenyl-1-butanone

Other names: 1,3-Diphenyl-1-butanone
1-Butanone, 1,3-diphenyl-
Inchi: InChI=1S/C16H16O/c1-13(14-8-4-2-5-9-14)12-16(17)15-10-6-3-7-11-15/h2-11,13H,12H2
InchiKey: GIVFXLVPKFXTCU-UHFFFAOYSA-N
Formula: C16H16O
SMILES: CC(CC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 224.30

Physical Properties

Property code	Value	Unit	Source
af	0.5174		Cheméo Relay (1.0)
gf	177.30	kJ/mol	Joback Method
hf	-20.27	kJ/mol	Cheméo Relay (1.0)
hfus	23.35	kJ/mol	Joback Method
hvap	89.98	kJ/mol	Cheméo Relay (1.0)
ie	8.71	eV	Cheméo Relay (1.0)
log10ws	-4.31		Cheméo Relay (1.0)
logp	4.063		Crippen Method
mcvol	190.350	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
tb	580.48	K	Cheméo Relay (1.0)
tc	849.22	K	Cheméo Relay (1.0)
tf	329.25	K	Cheméo Relay (1.0)
vc	0.683	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.92	J/mol×K	672.27	Joback Method
cpg	576.50	J/mol×K	913.58	Joback Method
cpg	565.41	J/mol×K	873.36	Joback Method
cpg	553.29	J/mol×K	833.14	Joback Method
cpg	540.07	J/mol×K	792.92	Joback Method
cpg	525.66	J/mol×K	752.71	Joback Method

cpg	509.97	J/mol×K	712.49	Joback Method
dvisc	0.0003870	Pa×s	515.06	Joback Method
dvisc	0.0001446	Pa×s	672.27	Joback Method
dvisc	0.0001900	Pa×s	619.87	Joback Method
dvisc	0.0002624	Pa×s	567.46	Joback Method
dvisc	0.0024590	Pa×s	357.85	Joback Method
dvisc	0.0006234	Pa×s	462.66	Joback Method
dvisc	0.0011342	Pa×s	410.25	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1533206&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

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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