

1,3-Diphenyl-2,4-pentanedione

Inchi:	InChI=1S/C17H16O2/c1-13(18)17(15-10-6-3-7-11-15)16(19)12-14-8-4-2-5-9-14/h2-11,17
InchiKey:	ZRPKYWOSTUYAPU-UHFFFAOYSA-N
Formula:	C17H16O2
SMILES:	CC(=O)C(C(=O)Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	252.31
CAS:	19588-08-0

Physical Properties

Property code	Value	Unit	Source
gf	56.80	kJ/mol	Joback Method
hf	-151.59	kJ/mol	Joback Method
hfus	27.54	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.171		Crippen Method
mcvol	206.010	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
tb	749.02	K	Joback Method
tc	990.71	K	Joback Method
tf	419.05	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.09	J/molxK	749.02	Joback Method
cpg	577.33	J/molxK	789.30	Joback Method
cpg	591.27	J/molxK	829.58	Joback Method
cpg	604.00	J/molxK	869.86	Joback Method
cpg	615.61	J/molxK	910.15	Joback Method
cpg	626.18	J/molxK	950.43	Joback Method
cpg	635.81	J/molxK	990.71	Joback Method
dvisc	0.0018128	Paxs	419.05	Joback Method
dvisc	0.0009053	Paxs	474.05	Joback Method

dvisc	0.0005223	Paxs	529.04	Joback Method
dvisc	0.0003342	Paxs	584.03	Joback Method
dvisc	0.0002309	Paxs	639.03	Joback Method
dvisc	0.0001692	Paxs	694.02	Joback Method
dvisc	0.0001298	Paxs	749.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19588080&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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