

1,6-Hexanedione, 1,6-diphenyl-

Other names:	Butane, 1,4-dibenzoyl- 1,4-Dibenzoylbutane 1,6-Diphenyl-1,6-hexanedione 1,6-diphenylhexane-1,6-dione
Inchi:	InChI=1S/C18H18O2/c19-17(15-9-3-1-4-10-15)13-7-8-14-18(20)16-11-5-2-6-12-16/h1-6,
InchiKey:	VRBLNWVVFVBNRK-UHFFFAOYSA-N
Formula:	C18H18O2
SMILES:	O=C(CCCCC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	266.33
CAS:	3375-38-0

Physical Properties

Property code	Value	Unit	Source
gf	67.66	kJ/mol	Joback Method
hf	-166.95	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	73.71	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.313		Crippen Method
mcvol	220.100	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
tb	772.34	K	Joback Method
tc	1005.29	K	Joback Method
tf	383.00 ± 3.00	K	NIST Webbook
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.82	J/mol×K	772.34	Joback Method
cpg	631.01	J/mol×K	811.17	Joback Method
cpg	644.98	J/mol×K	849.99	Joback Method
cpg	657.80	J/mol×K	888.82	Joback Method
cpg	669.57	J/mol×K	927.64	Joback Method

cpg	680.36	J/mol×K	966.47	Joback Method
cpg	690.25	J/mol×K	1005.29	Joback Method
dvisc	0.0014296	Pa×s	445.32	Joback Method
dvisc	0.0007629	Pa×s	499.82	Joback Method
dvisc	0.0004607	Pa×s	554.33	Joback Method
dvisc	0.0003045	Pa×s	608.83	Joback Method
dvisc	0.0002154	Pa×s	663.33	Joback Method
dvisc	0.0001606	Pa×s	717.84	Joback Method
dvisc	0.0001248	Pa×s	772.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3375380&Units=SI
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

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/24-654-9/1-6-Hexanedione-1-6-diphenyl.pdf>

Generated by Cheméo on 2025-12-23 02:23:11.65882162 +0000 UTC m=+6204789.188862278.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.