1,6-DIPHENYLHEXANE-1,6-DIONE

Other names: 1,4-Dibenzoylbutane
1,6-Diphenyl-1,6-hexanedione
1,6-diphenylhexane-1,6-dione
Butane, 1,4-dibenzoyl-
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]: 266.34

Physical Properties

Property code	Value	Unit	Source
af	0.7160		Cheméo Relay (1.0)
gf	67.66	kJ/mol	Joback Method
hf	-182.88	kJ/mol	Cheméo Relay (1.0)
hfus	33.66	kJ/mol	Joback Method
hvap	108.56	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
log10ws	-4.74		Cheméo Relay (1.0)
logp	4.313		Crippen Method
mcvol	220.100	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
tb	636.38	K	Cheméo Relay (1.0)
tc	900.18	K	Cheméo Relay (1.0)
tf	383.00 ± 3.00	K	NIST Webbook
vc	0.813	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.82	J/mol×K	772.34	Joback Method
cpg	690.25	J/mol×K	1005.29	Joback Method
cpg	680.36	J/mol×K	966.47	Joback Method
cpg	669.57	J/mol×K	927.64	Joback Method

cpg	657.80	J/mol×K	888.82	Joback Method
cpg	644.98	J/mol×K	849.99	Joback Method
cpg	631.01	J/mol×K	811.17	Joback Method
dvisc	0.0003045	Pa×s	608.83	Joback Method
dvisc	0.0001248	Pa×s	772.34	Joback Method
dvisc	0.0001606	Pa×s	717.84	Joback Method
dvisc	0.0002154	Pa×s	663.33	Joback Method
dvisc	0.0014296	Pa×s	445.32	Joback Method
dvisc	0.0004607	Pa×s	554.33	Joback Method
dvisc	0.0007629	Pa×s	499.82	Joback Method

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3375380&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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