Dibenzoylmethane

Other names:	1,3-Propanedione, 1,3-diphenyl- «omega»-Benzoylacetophenone Phenyl phenacyl ketone 1,3-Diphenyl-1,3-propanedione 2-Benzoylacetophenone 1,3-Diphenylpropane-1,3-dione omega-Benzoylacetophenone Karenzu DK 2 Rhodiastab 83 NSC 6266
Inchi:	InChI=1S/C15H12O2/c16-14(12-7-3-1-4-8-12)11-15(17)13-9-5-2-6-10-13/h1-10H,11H2
InchiKey:	NZZIMKJIVMHWJC-UHFFFAOYSA-N
Formula:	C15H12O2
SMILES:	O=C(CC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	224.25
CAS:	120-46-7

Physical Properties

Property code	Value	Unit	Source
chs	-7386.00 ± 4.60	kJ/mol	NIST Webbook
chs	-7395.00 ± 3.00	kJ/mol	NIST Webbook
chs	-7410.00	kJ/mol	NIST Webbook
chs	-7393.00 ± 2.00	kJ/mol	NIST Webbook
gf	42.40	kJ/mol	Joback Method
hf	-109.20 ± 2.00	kJ/mol	NIST Webbook
hfs	-228.00 ± 12.00	kJ/mol	NIST Webbook
hfs	-222.30	kJ/mol	NIST Webbook
hfs	-241.00	kJ/mol	NIST Webbook
hfus	25.89	kJ/mol	Joback Method
hsub	113.30 ± 4.80	kJ/mol	NIST Webbook
hsub	50.20	kJ/mol	NIST Webbook
hsub	115.70 ± 0.90	kJ/mol	NIST Webbook
hsub	115.70 ± 0.90	kJ/mol	NIST Webbook
hvap	67.03	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.45 ± 0.05	eV	NIST Webbook
log10ws	-4.02		Crippen Method

logp	3.142		Crippen Method
mcvol	177.830	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	703.70	K	Joback Method
tc	950.85	K	Joback Method
tf	351.00 ± 3.00	K	NIST Webbook
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.25	J/mol×K	703.70	Joback Method
cpg	470.52	J/mol×K	744.89	Joback Method
cpg	483.54	J/mol×K	786.08	Joback Method
cpg	495.38	J/mol×K	827.27	Joback Method
cpg	506.14	J/mol×K	868.46	Joback Method
cpg	515.89	J/mol×K	909.66	Joback Method
cpg	524.72	J/mol×K	950.85	Joback Method
dvisc	0.0017667	Pa×s	411.51	Joback Method
dvisc	0.0009825	Pa×s	460.21	Joback Method
dvisc	0.0006113	Pa×s	508.91	Joback Method
dvisc	0.0004132	Pa×s	557.61	Joback Method
dvisc	0.0002974	Pa×s	606.30	Joback Method
dvisc	0.0002248	Pa×s	655.00	Joback Method
dvisc	0.0001767	Pa×s	703.70	Joback Method
hvapt	60.10	kJ/mol	375.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	493.20	K	2.40	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120467&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume