2-Butene-1,4-dione, 1,4-diphenyl-

Other names:	Ethylene, 1,2-dibenzoyl-
	Dibenzoylethylene
	1,2-Dibenzoylethylene
	1,4-Diphenyl-2-butene-1,4-dione
	USAF nd-57
	1,2-Dibenzoylethene
	1,4-diphenylbut-2-ene-1,4-dione
Inchi:	InChI=1S/C16H12O2/c17-15(13-7-3-1-4-8-13)11-12-16(18)14-9-5-2-6-10-14/h1-12H
InchiKey:	WYCXGQSQHAXLPK-UHFFFAOYSA-N
Formula:	C16H12O2
SMILES:	O=C(C=CC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	236.27
CAS:	4070-75-1

Physical Properties

Property code	Value	Unit	Source
chs	-7896.50 ± 2.30	kJ/mol	NIST Webbook
gf	131.04	kJ/mol	Joback Method
hf	-8.45	kJ/mol	Joback Method
hfs	-114.70 ± 2.40	kJ/mol	NIST Webbook
hfus	28.68	kJ/mol	Joback Method
hvap	69.21	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.308		Crippen Method
mcvol	187.620	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
ss	319.20	J/mol×K	NIST Webbook
tb	730.74	K	Joback Method
tc	982.37	K	Joback Method
tf	417.70	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.05	J/mol×K	730.74	Joback Method
cpg	498.05	J/mol×K	772.68	Joback Method
cpg	510.80	J/mol×K	814.62	Joback Method
cpg	522.42	J/mol×K	856.56	Joback Method
cpg	533.02	J/mol×K	898.50	Joback Method
cpg	542.73	J/mol×K	940.43	Joback Method
cpg	551.65	J/mol×K	982.37	Joback Method
cps	286.60	J/mol×K	291.90	NIST Webbook
dvisc	0.0015260	Pa×s	417.70	Joback Method
dvisc	0.0008165	Pa×s	469.87	Joback Method
dvisc	0.0004951	Pa×s	522.05	Joback Method
dvisc	0.0003287	Pa×s	574.22	Joback Method
dvisc	0.0002337	Pa×s	626.39	Joback Method
dvisc	0.0001751	Pa×s	678.57	Joback Method
dvisc	0.0001367	Pa×s	730.74	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4070751&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

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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
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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume