trans-1,2-Dibenzoylethylene

Other names:	2-Butene-1,4-dione, 1,4-diphenyl-, (E)- trans-1,4-Diphenyl-2-butene-1,4-dione (E)-1,4-diphenyl-2-butene-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/b12
InchiKey:	WYCXGQSQHAXLPK-VAWYXSNFSA-N
Formula:	C16H12O2
SMILES:	O=C(C=CC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	236.27
CAS:	959-28-4

Physical Properties

Property code	Value	Unit	Source
gf	131.04	kJ/mol	Joback Method
hf	-8.45	kJ/mol	Joback Method
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
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
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

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=C959284&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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