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: 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=C959284&Units=SI

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