

4,4'-Diacetyl biphenyl

Inchi:	InChI=1S/C16H14O2/c1-11(17)13-3-7-15(8-4-13)16-9-5-14(6-10-16)12(2)18/h3-10H,1-2H
InchiKey:	YSTSBXDVNKYPTR-UHFFFAOYSA-N
Formula:	C16H14O2
SMILES:	CC(=O)c1ccc(-c2ccc(C(C)=O)cc2)cc1
Mol. weight [g/mol]:	238.28
CAS:	787-69-9

Physical Properties

Property code	Value	Unit	Source
gf	31.56	kJ/mol	Joback Method
hf	-148.61	kJ/mol	Joback Method
hfus	27.70	kJ/mol	Joback Method
hvap	70.58	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.759		Crippen Method
mcvol	191.920	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
tb	736.54	K	Joback Method
tc	980.06	K	Joback Method
tf	447.82	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.86	J/molxK	736.54	Joback Method
cpg	566.45	J/molxK	939.47	Joback Method
cpg	556.44	J/molxK	898.89	Joback Method
cpg	545.44	J/molxK	858.30	Joback Method
cpg	533.38	J/molxK	817.71	Joback Method
cpg	520.21	J/molxK	777.13	Joback Method
cpg	575.54	J/molxK	980.06	Joback Method
dvisc	0.0001589	Paxs	736.54	Joback Method
dvisc	0.0001971	Paxs	688.42	Joback Method

dvisc	0.0002526	Paxs	640.30	Joback Method
dvisc	0.0003371	Paxs	592.18	Joback Method
dvisc	0.0004735	Paxs	544.06	Joback Method
dvisc	0.0007102	Paxs	495.94	Joback Method
dvisc	0.0011624	Paxs	447.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C787699&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
mccvol:	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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