

trans,trans-Dibenzylideneacetone

Other names:	1,4-Pentadien-3-one, 1,5-diphenyl-, (1E,4E)-dibenzylideneacetone
Inchi:	InChI=1S/C17H14O/c18-17(13-11-15-7-3-1-4-8-15)14-12-16-9-5-2-6-10-16/h1-14H/b13-
InchiKey:	WMKGGPCROCCUDY-PHEQNACWSA-N
Formula:	C17H14O
SMILES:	O=C(C=Cc1ccccc1)C=Cc1ccccc1
Mol. weight [g/mol]:	234.29
CAS:	35225-79-7

Physical Properties

Property code	Value	Unit	Source
gf	348.60	kJ/mol	Joback Method
hf	200.71	kJ/mol	Joback Method
hfus	29.87	kJ/mol	Joback Method
hvap	64.65	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.982		Crippen Method
mvol	195.840	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
tb	703.91	K	Joback Method
tc	954.96	K	Joback Method
tf	373.96	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.70	J/molxK	703.91	Joback Method
cpg	514.49	J/molxK	745.75	Joback Method
cpg	528.96	J/molxK	787.59	Joback Method
cpg	542.24	J/molxK	829.43	Joback Method
cpg	554.49	J/molxK	871.27	Joback Method
cpg	565.84	J/molxK	913.11	Joback Method
cpg	576.44	J/molxK	954.96	Joback Method

dvisc	0.0015983	Paxs	373.96	Joback Method
dvisc	0.0007579	Paxs	428.95	Joback Method
dvisc	0.0004258	Paxs	483.94	Joback Method
dvisc	0.0002691	Paxs	538.93	Joback Method
dvisc	0.0001851	Paxs	593.93	Joback Method
dvisc	0.0001357	Paxs	648.92	Joback Method
dvisc	0.0001044	Paxs	703.91	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=C35225797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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