

2-Buten-1-one, 1,3-diphenyl-

Other names:	Chalcone, «beta»-methyl- «beta»-Methylchalcone Dyprnone 1,3-Diphenyl-2-buten-1-one
Inchi:	InChI=1S/C16H14O/c1-13(14-8-4-2-5-9-14)12-16(17)15-10-6-3-7-11-15/h2-12H,1H3/b13
InchiKey:	PLELHVCQAU LGBH-OUKQBFOZSA-N
Formula:	C16H14O
SMILES:	<chem>CC(=CC(=O)c1ccccc1)c1ccccc1</chem>
Mol. weight [g/mol]:	222.28
CAS:	495-45-4

Physical Properties

Property code	Value	Unit	Source
gf	251.41	kJ/mol	Joback Method
hf	94.34	kJ/mol	Joback Method
hfus	25.77	kJ/mol	Joback Method
hvap	62.55	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.973		Crippen Method
mcvol	186.050	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1985.70		NIST Webbook
tb	615.70	K	NIST Webbook
tc	927.48	K	Joback Method
tf	353.81	K	Joback Method
vc	0.703	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.61	J/mol×K	676.75	Joback Method
cpg	485.92	J/mol×K	718.54	Joback Method
cpg	500.86	J/mol×K	760.33	Joback Method
cpg	514.55	J/mol×K	802.12	Joback Method

cpg	527.10	J/mol×K	843.91	Joback Method
cpg	538.62	J/mol×K	885.69	Joback Method
cpg	549.25	J/mol×K	927.48	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	479.50 ± 0.50	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C495454&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

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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