

6-phenylhexa-3,5-dien-2-one

Inchi:	InChI=1S/C12H12O/c1-11(13)7-5-6-10-12-8-3-2-4-9-12/h2-10H,1H3/b7-5+,10-6+
InchiKey:	PRNUCJKOERXADE-YLNKAEQOSA-N
Formula:	C12H12O
SMILES:	CC(=O)C=CC=Cc1ccccc1
Mol. weight [g/mol]:	172.22
CAS:	4173-44-8

Physical Properties

Property code	Value	Unit	Source
gf	194.09	kJ/mol	Joback Method
hf	67.38	kJ/mol	Joback Method
hfus	22.88	kJ/mol	Joback Method
hvap	51.24	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.845		Crippen Method
mcvol	149.150	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1655.90		NIST Webbook
tb	562.83	K	Joback Method
tc	790.32	K	Joback Method
tf	291.19	K	Joback Method
vc	0.566	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.19	J/molxK	562.83	Joback Method
cpg	392.75	J/molxK	752.41	Joback Method
cpg	382.06	J/molxK	714.49	Joback Method
cpg	370.53	J/molxK	676.58	Joback Method
cpg	358.10	J/molxK	638.66	Joback Method
cpg	344.68	J/molxK	600.75	Joback Method
cpg	402.70	J/molxK	790.32	Joback Method
dvisc	0.0001638	Paxs	562.83	Joback Method

dvisc	0.0002125	Paxs	517.56	Joback Method
dvisc	0.0002896	Paxs	472.28	Joback Method
dvisc	0.0004216	Paxs	427.01	Joback Method
dvisc	0.0006708	Paxs	381.74	Joback Method
dvisc	0.0012095	Paxs	336.46	Joback Method
dvisc	0.0026197	Paxs	291.19	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=C4173448&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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