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=C/C=C/c1ccccc1
Mol. weight [g/mol]: 172.23

Physical Properties

Property code	Value	Unit	Source
hf	13.86	kJ/mol	Cheméo Relay (1.0)
hfus	22.88	kJ/mol	Joback Method
hvap	72.73	kJ/mol	Cheméo Relay (1.0)
ie	8.07	eV	Cheméo Relay (1.0)
log10ws	-3.21		Cheméo Relay (1.0)
logp	2.845		Crippen Method
mcvol	149.150	ml/mol	McGowan Method
rinpol	1655.90		NIST Webbook
tb	563.61	K	Cheméo Relay (1.0)
tf	385.60	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.19	J/mol×K	562.83	Joback Method
cpg	402.70	J/mol×K	790.32	Joback Method
cpg	392.75	J/mol×K	752.41	Joback Method
cpg	382.06	J/mol×K	714.49	Joback Method
cpg	370.53	J/mol×K	676.58	Joback Method
cpg	358.10	J/mol×K	638.66	Joback Method
cpg	344.68	J/mol×K	600.75	Joback Method
dvisc	0.0004216	Pa×s	427.01	Joback Method
dvisc	0.0001638	Pa×s	562.83	Joback Method
dvisc	0.0002125	Pa×s	517.56	Joback Method
dvisc	0.0002896	Pa×s	472.28	Joback Method
dvisc	0.0026197	Pa×s	291.19	Joback Method

dvisc	0.0006708	Pa×s	381.74	Joback Method
dvisc	0.0012095	Pa×s	336.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4173448&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point