5-METHYL-1-PHENYLHEXA-1,3,4-TRIENE

Inchi: InChI=1S/C13H14/c1-12(2)8-6-7-11-13-9-4-3-5-10-13/h3-7,9-11H,1-2H3/b11-7+
InchiKey: ODCHZOADCIUBBE-YRNVUSSQSA-N
Formula: C13H14
SMILES: CC(C)=C=C/C=C/c1ccccc1
Mol. weight [g/mol]: 170.26

Physical Properties

Property code	Value	Unit	Source
hf	291.82	kJ/mol	Cheméo Relay (1.0)
hfus	24.69	kJ/mol	Joback Method
hvap	61.38	kJ/mol	Cheméo Relay (1.0)
ie	7.85	eV	Cheméo Relay (1.0)
logp	3.821		Crippen Method
mcvol	157.370	ml/mol	McGowan Method
tb	532.90	K	Cheméo Relay (1.0)
tf	343.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.18	J/mol×K	534.99	Joback Method
cpg	357.78	J/mol×K	573.74	Joback Method
cpg	373.25	J/mol×K	612.48	Joback Method
cpg	387.64	J/mol×K	651.23	Joback Method
cpg	401.04	J/mol×K	689.97	Joback Method
cpg	413.52	J/mol×K	728.72	Joback Method
cpg	425.15	J/mol×K	767.46	Joback Method

Sources

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=C103240795&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point