

5-Phenylbicyclo(2.2.1)2-heptene

Inchi:	InChI=1S/C13H14/c1-2-4-11(5-3-1)13-9-10-6-7-12(13)8-10/h1-7,10,12-13H,8-9H2
InchiKey:	PGNNHYNYFLXKDZ-UHFFFAOYSA-N
Formula:	C13H14
SMILES:	C1=CC2CC1CC2c1ccccc1
Mol. weight [g/mol]:	170.26

Physical Properties

Property code	Value	Unit	Source
hfus	19.93	kJ/mol	Joback Method
ie	8.24	eV	Cheméo Relay (1.0)
logp	3.366		Crippen Method
mcvol	144.250	ml/mol	McGowan Method
tb	518.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.64	J/mol×K	535.76	Joback Method
cpg	447.79	J/mol×K	774.95	Joback Method
cpg	434.43	J/mol×K	735.08	Joback Method
cpg	419.97	J/mol×K	695.22	Joback Method
cpg	404.27	J/mol×K	655.35	Joback Method
cpg	387.24	J/mol×K	615.49	Joback Method
cpg	368.73	J/mol×K	575.62	Joback Method
dvisc	0.0009802	Pa×s	413.67	Joback Method
dvisc	0.0007836	Pa×s	535.76	Joback Method
dvisc	0.0008340	Pa×s	495.06	Joback Method
dvisc	0.0008976	Pa×s	454.36	Joback Method
dvisc	0.0014787	Pa×s	291.57	Joback Method
dvisc	0.0010910	Pa×s	372.97	Joback Method
dvisc	0.0012467	Pa×s	332.27	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=C6143302&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
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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