

6-[(Z)-1-BUTENYL]-1,4-CYCLOHEPTADIENE

Other names:	6-[(1Z)-1-Butenyl]-1,4-cycloheptadiene Ectocarpene
Inchi:	InChI=1S/C11H16/c1-2-3-8-11-9-6-4-5-7-10-11/h3-4,6-8,10-11H,2,5,9H2,1H3/b8-3-
InchiKey:	KIFXGGYCNMHCSX-BAQGIRSFSA-N
Formula:	C11H16
SMILES:	CC/C=C\C1C=CCC=CC1
Mol. weight [g/mol]:	148.25

Physical Properties

Property code	Value	Unit	Source
hfus	16.63	kJ/mol	Joback Method
logp	3.475		Crippen Method
mcvol	142.090	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.77	J/mol×K	477.38	Joback Method
cpg	317.60	J/mol×K	513.44	Joback Method
cpg	335.31	J/mol×K	549.49	Joback Method
cpg	351.96	J/mol×K	585.55	Joback Method
cpg	367.57	J/mol×K	621.61	Joback Method
cpg	382.21	J/mol×K	657.67	Joback Method
cpg	395.90	J/mol×K	693.72	Joback Method
dvisc	0.0074717	Pa×s	214.03	Joback Method
dvisc	0.0023244	Pa×s	257.92	Joback Method
dvisc	0.0010156	Pa×s	301.81	Joback Method
dvisc	0.0005475	Pa×s	345.71	Joback Method
dvisc	0.0003393	Pa×s	389.60	Joback Method
dvisc	0.0002316	Pa×s	433.49	Joback Method
dvisc	0.0001696	Pa×s	477.38	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=C33156933&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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