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: CCC=CC1C=CCC=CC1
Mol. weight [g/mol]: 148.24
CAS: 33156-93-3

Physical Properties

Property code	Value	Unit	Source
gf	194.23	kJ/mol	Joback Method
hf	10.57	kJ/mol	Joback Method
hfus	16.63	kJ/mol	Joback Method
hvap	41.22	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.475		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
tb	477.38	K	Joback Method
tc	693.72	K	Joback Method
tf	214.03	K	Joback Method
vc	0.528	m3/kmol	Joback 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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C33156933&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume