

Endo-5-vinylbicyclo[2.2.1]hept-2-ene

Inchi: InChI=1S/C9H12/c1-2-8-5-7-3-4-9(8)6-7/h2-4,7-9H,1,5-6H2/t??,8-,9?/m0/s1
InchiKey: INYHZQLKOKTDAI-MGURRDGZSA-N
Formula: C9H12
SMILES: C=CC1CC2C=CC1C2
Mol. weight [g/mol]: 120.19
CAS: 117110-17-5

Physical Properties

Property code	Value	Unit	Source
chl	-5371.40 ± 1.60	kJ/mol	NIST Webbook
gf	244.39	kJ/mol	Joback Method
hf	157.00 ± 2.00	kJ/mol	NIST Webbook
hfl	114.80 ± 1.70	kJ/mol	NIST Webbook
hfus	14.25	kJ/mol	Joback Method
hvap	42.20	kJ/mol	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.385		Crippen Method
mcvol	107.350	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	414.24	K	Joback Method
tc	619.79	K	Joback Method
tf	218.31	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.72	J/molxK	414.24	Joback Method
cpg	286.28	J/molxK	585.54	Joback Method
cpg	273.51	J/molxK	551.28	Joback Method
cpg	259.84	J/molxK	517.02	Joback Method
cpg	245.19	J/molxK	482.76	Joback Method
cpg	229.50	J/molxK	448.50	Joback Method
cpg	298.20	J/molxK	619.79	Joback Method

dvisc	0.0004967	Paxs	414.24	Joback Method
dvisc	0.0004897	Paxs	381.59	Joback Method
dvisc	0.0004814	Paxs	348.93	Joback Method
dvisc	0.0004717	Paxs	316.27	Joback Method
dvisc	0.0004600	Paxs	283.62	Joback Method
dvisc	0.0004456	Paxs	250.97	Joback Method
dvisc	0.0004277	Paxs	218.31	Joback Method

Sources

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=C117110175&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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