Exo-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
InchiKey: INYHZQLKOKTDAI-UHFFFAOYSA-N
Formula: C9H12
SMILES: C=CC1CC2C=CC1C2
Mol. weight [g/mol]: 120.19
CAS: 25093-48-5

Physical Properties

Property code	Value	Unit	Source
chl	-5371.40	kJ/mol	NIST Webbook
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
hf	157.00 ± 2.00	kJ/mol	NIST Webbook
hfl	114.80 ± 1.70	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/mol×K	414.24	Joback Method
cpg	229.50	J/mol×K	448.50	Joback Method
cpg	245.19	J/mol×K	482.76	Joback Method
cpg	259.84	J/mol×K	517.02	Joback Method

cpg	273.51	J/mol×K	551.28	Joback Method
cpg	286.28	J/mol×K	585.54	Joback Method
cpg	298.20	J/mol×K	619.79	Joback Method
dvisc	0.0004277	Pa×s	218.31	Joback Method
dvisc	0.0004456	Pa×s	250.97	Joback Method
dvisc	0.0004600	Pa×s	283.62	Joback Method
dvisc	0.0004717	Pa×s	316.27	Joback Method
dvisc	0.0004814	Pa×s	348.93	Joback Method
dvisc	0.0004897	Pa×s	381.59	Joback Method
dvisc	0.0004967	Pa×s	414.24	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=C25093485&Units=SI

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