

Anti-tricyclo[3.2.0.0(2,4)]hept-6-ene

Inchi:	InChI=1S/C7H8/c1-2-5-4(1)6-3-7(5)6/h1-2,4-7H,3H2
InchiKey:	DLJZNMLNAZRUIH-UHFFFAOYSA-N
Formula:	C7H8
SMILES:	C1=CC2C1C1CC21
Mol. weight [g/mol]:	92.14
CAS:	79356-83-5

Physical Properties

Property code	Value	Unit	Source
gf	236.76	kJ/mol	Joback Method
hf	383.90	kJ/mol	NIST Webbook
hfus	14.78	kJ/mol	Joback Method
hvap	30.55	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.438		Crippen Method
mcvol	72.610	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
tb	365.73	K	Joback Method
tc	561.87	K	Joback Method
tf	226.03	K	Joback Method
vc	0.299	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.21	J/mol×K	365.73	Joback Method
cpg	198.00	J/mol×K	529.18	Joback Method
cpg	187.89	J/mol×K	496.49	Joback Method
cpg	176.83	J/mol×K	463.80	Joback Method
cpg	164.76	J/mol×K	431.11	Joback Method
cpg	151.58	J/mol×K	398.42	Joback Method
cpg	207.27	J/mol×K	561.87	Joback Method
dvisc	0.0005194	Pa×s	365.73	Joback Method
dvisc	0.0004042	Pa×s	342.45	Joback Method

dvisc	0.0003033	Pa×s	319.16	Joback Method
dvisc	0.0002175	Pa×s	295.88	Joback Method
dvisc	0.0001474	Pa×s	272.60	Joback Method
dvisc	0.0000929	Pa×s	249.31	Joback Method
dvisc	0.0000532	Pa×s	226.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79356835&Units=SI
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

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

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