

Tetracyclo[4.1.0.0(2,4).0(3,5)]heptane

Inchi:	InChI=1S/C7H8/c1-2-3(1)5-6-4(2)7(5)6/h2-7H,1H2
InchiKey:	QBLIOMUVZBDTLW-UHFFFAOYSA-N
Formula:	C7H8
SMILES:	C1C2C1C1C3C2C13
Mol. weight [g/mol]:	92.14
CAS:	50861-26-2

Physical Properties

Property code	Value	Unit	Source
gf	296.14	kJ/mol	Joback Method
hf	370.00	kJ/mol	NIST Webbook
hfus	19.07	kJ/mol	Joback Method
hvap	29.35	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	1.128		Crippen Method
mcvol	66.050	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	355.83	K	Joback Method
tc	541.30	K	Joback Method
tf	249.53	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.29	J/mol×K	355.83	Joback Method
cpg	200.66	J/mol×K	510.39	Joback Method
cpg	190.29	J/mol×K	479.47	Joback Method
cpg	178.87	J/mol×K	448.56	Joback Method
cpg	166.29	J/mol×K	417.65	Joback Method
cpg	152.46	J/mol×K	386.74	Joback Method
cpg	210.09	J/mol×K	541.30	Joback Method
dvisc	0.0005902	Pa×s	355.83	Joback Method
dvisc	0.0003992	Pa×s	338.11	Joback Method

dvisc	0.0002585	Pa×s	320.40	Joback Method
dvisc	0.0001591	Pa×s	302.68	Joback Method
dvisc	0.0000922	Pa×s	284.96	Joback Method
dvisc	0.0000497	Pa×s	267.25	Joback Method
dvisc	0.0000245	Pa×s	249.53	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=C50861262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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