

trans Bicyclo[6.1.0]nona-2,4,6-triene

Inchi: InChI=1S/C9H10/c1-2-4-6-9-7-8(9)5-3-1/h1-6,8-9H,7H2/b2-1-,5-3-,6-4-
InchiKey: ZMCCSKLGOXNRGF-XCADPSHZSA-N
Formula: C9H10
SMILES: C1=CC=CC2CC2C=C1
Mol. weight [g/mol]: 118.18
CAS: 18012-46-9

Physical Properties

Property code	Value	Unit	Source
gf	199.98	kJ/mol	Joback Method
hf	372.00	kJ/mol	NIST Webbook
hfus	12.70	kJ/mol	Joback Method
hvap	36.85	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.305		Crippen Method
mcvol	103.050	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	429.09	K	Joback Method
tc	652.42	K	Joback Method
tf	218.79	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.74	J/mol×K	429.09	Joback Method
cpg	269.90	J/mol×K	615.20	Joback Method
cpg	257.76	J/mol×K	577.98	Joback Method
cpg	244.63	J/mol×K	540.76	Joback Method
cpg	230.47	J/mol×K	503.53	Joback Method
cpg	215.19	J/mol×K	466.31	Joback Method
cpg	281.14	J/mol×K	652.42	Joback Method
dvisc	0.0004011	Pa×s	429.09	Joback Method
dvisc	0.0004429	Pa×s	394.04	Joback Method

dvisc	0.0004987	Pa×s	358.99	Joback Method
dvisc	0.0005762	Pa×s	323.94	Joback Method
dvisc	0.0006894	Pa×s	288.89	Joback Method
dvisc	0.0008668	Pa×s	253.84	Joback Method
dvisc	0.0011728	Pa×s	218.79	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=C18012469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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