

Tricyclo[7.2.1.0(5,12)]dodecane, isomer # 1

Inchi: InChI=1S/C12H20/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h9-12H,1-8H2
InchiKey: FZDZWLDRELLWNN-UHFFFAOYSA-N
Formula: C12H20
SMILES: C1CC2CCCC3CCC(C1)C23
Mol. weight [g/mol]: 164.29

Physical Properties

Property code	Value	Unit	Source
gf	188.40	kJ/mol	Joback Method
hf	-111.43	kJ/mol	Joback Method
hfus	16.01	kJ/mol	Joback Method
hvap	42.25	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.613		Crippen Method
mcvol	147.360	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1291.00		NIST Webbook
ripol	1462.00		NIST Webbook
ripol	1430.00		NIST Webbook
tb	502.32	K	Joback Method
tc	726.21	K	Joback Method
tf	264.02	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.20	J/molxK	502.32	Joback Method
cpg	393.61	J/molxK	539.63	Joback Method
cpg	416.37	J/molxK	576.95	Joback Method
cpg	437.59	J/molxK	614.26	Joback Method
cpg	457.35	J/molxK	651.58	Joback Method
cpg	475.77	J/molxK	688.89	Joback Method

cpg	492.92	J/mol×K	726.21	Joback Method
dvisc	0.0016617	Paxs	264.02	Joback Method
dvisc	0.0014428	Paxs	303.74	Joback Method
dvisc	0.0012943	Paxs	343.45	Joback Method
dvisc	0.0011875	Paxs	383.17	Joback Method
dvisc	0.0011073	Paxs	422.89	Joback Method
dvisc	0.0010450	Paxs	462.60	Joback Method
dvisc	0.0009953	Paxs	502.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R524473&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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