

Tricyclo[7.2.1.0(5,12)]dodecane, isomer # 4

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	1344.00		NIST Webbook
rinpol	1323.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1504.00		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/mol×K	502.32	Joback Method
cpg	475.77	J/mol×K	688.89	Joback Method
cpg	457.35	J/mol×K	651.58	Joback Method
cpg	437.59	J/mol×K	614.26	Joback Method
cpg	416.37	J/mol×K	576.95	Joback Method

cpg	393.61	J/mol×K	539.63	Joback Method
cpg	492.92	J/mol×K	726.21	Joback Method
dvisc	0.0009953	Pa×s	502.32	Joback Method
dvisc	0.0010450	Pa×s	462.60	Joback Method
dvisc	0.0011073	Pa×s	422.89	Joback Method
dvisc	0.0011875	Pa×s	383.17	Joback Method
dvisc	0.0012943	Pa×s	343.45	Joback Method
dvisc	0.0014428	Pa×s	303.74	Joback Method
dvisc	0.0016617	Pa×s	264.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R524502&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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