

Tricyclo[5.2.1.0(2.6)]deca-3,8-diene, 4,7-dimethyl

Inchi:	InChI=1S/C12H16/c1-8-5-10-9-3-4-12(2,7-9)11(10)6-8/h3-5,9-11H,6-7H2,1-2H3
InchiKey:	MOOJGAKRRUPYKX-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	CC1=CC2C3C=CC(C)(C3)C2C1
Mol. weight [g/mol]:	160.26

Physical Properties

Property code	Value	Unit	Source
gf	257.40	kJ/mol	Joback Method
hf	20.22	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	42.00	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.165		Crippen Method
mcvol	138.760	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	497.32	K	Joback Method
tc	719.64	K	Joback Method
tf	309.00	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.53	J/mol×K	497.32	Joback Method
cpg	354.90	J/mol×K	534.37	Joback Method
cpg	372.68	J/mol×K	571.43	Joback Method
cpg	389.05	J/mol×K	608.48	Joback Method
cpg	404.23	J/mol×K	645.54	Joback Method
cpg	418.42	J/mol×K	682.59	Joback Method
cpg	431.80	J/mol×K	719.64	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=R298149&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
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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