Tricyclo[5.2.1.0(2.6)]deca-3,8-diene, 1,4-dimethyl

Inchi: InChI=1S/C12H16/c1-8-5-10-9-3-4-12(2,7-9)11(10)6-8/h3-4,6,9-11H,5,7H2,1-2H3
InchiKey: LQCOQEHQUPKMBA-UHFFFAOYSA-N
Formula: C12H16
SMILES: CC1=CC2C(C1)C1C=CC2(C)C1
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
rinpol	1086.70		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1079.50		NIST Webbook
rinpol	1121.40		NIST Webbook
rinpol	1111.10		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1111.10		NIST Webbook
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=R298109&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume