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

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

Physical Properties

Property code	Value	Unit	Source
gf	253.26	kJ/mol	Joback Method
hf	-6.49	kJ/mol	Joback Method
hfus	21.88	kJ/mol	Joback Method
hvap	43.82	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.165		Crippen Method
mcvol	138.760	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1134.00		NIST Webbook
rinpol	1136.80		NIST Webbook
rinpol	1146.40		NIST Webbook
rinpol	1100.20		NIST Webbook
rinpol	1107.60		NIST Webbook
rinpol	1124.00		NIST Webbook
tb	502.06	K	Joback Method
tc	716.34	K	Joback Method
tf	297.62	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.26	J/mol×K	502.06	Joback Method
cpg	355.11	J/mol×K	537.77	Joback Method
cpg	372.70	J/mol×K	573.49	Joback Method
cpg	389.11	J/mol×K	609.20	Joback Method

cpg	404.44	J/mol×K	644.91	Joback Method
cpg	418.78	J/mol×K	680.63	Joback Method
cpg	432.21	J/mol×K	716.34	Joback Method
dvisc	0.0007477	Pa×s	297.62	Joback Method
dvisc	0.0008690	Pa×s	331.69	Joback Method
dvisc	0.0009820	Pa×s	365.77	Joback Method
dvisc	0.0010869	Pa×s	399.84	Joback Method
dvisc	0.0011839	Pa×s	433.91	Joback Method
dvisc	0.0012737	Pa×s	467.99	Joback Method
dvisc	0.0013567	Pa×s	502.06	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R298154&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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