Germacrene D isomer # 1

Other names: 1-Methyl-5-methylene-8-(1-methylethyl)-1,6-cyclodecadiene
Inchi: InChI=1S/C15H24/c1-12(2)15-10-8-13(3)6-5-7-14(4)9-11-15/h7-8,10,12,15H,3,5-6,9,11H
InchiKey: GAIBLDCXCZKKJE-YZJXYJLZSA-N
Formula: C15H24
SMILES: C=C1C=CC(C(C)C)CCC(C)=CCC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	152.40	kJ/mol	Joback Method
hf	-140.20	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.891		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	581.25	K	Joback Method
tc	804.50	K	Joback Method
tf	264.83	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.53	J/mol×K	581.25	Joback Method
cpg	523.14	J/mol×K	618.46	Joback Method
cpg	545.41	J/mol×K	655.67	Joback Method
cpg	566.34	J/mol×K	692.88	Joback Method
cpg	585.93	J/mol×K	730.09	Joback Method
cpg	604.19	J/mol×K	767.29	Joback Method

cpg	621.12	J/mol×K	804.50	Joback Method
dvisc	0.0085131	Pa×s	264.83	Joback Method
dvisc	0.0019587	Pa×s	317.57	Joback Method
dvisc	0.0006848	Pa×s	370.30	Joback Method
dvisc	0.0003112	Pa×s	423.04	Joback Method
dvisc	0.0001684	Pa×s	475.78	Joback Method
dvisc	0.0001030	Pa×s	528.51	Joback Method
dvisc	0.0000689	Pa×s	581.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R286314&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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