Geijerene

Other names: 2-Isopropenyl-1-methyl-1-vinyl-3-cyclohexane
Inchi: InChI=1S/C12H18/c1-5-12(4)9-7-6-8-11(12)10(2)3/h5-6,8,11H,1-2,7,9H2,3-4H3
InchiKey: BGDQCKOAZKTOFV-UHFFFAOYSA-N
Formula: C12H18
SMILES: C=CC1(C)CCC=CC1C(=C)C
Mol. weight [g/mol]: 162.27
CAS: 6902-73-4

Physical Properties

Property code	Value	Unit	Source
gf	258.50	kJ/mol	Joback Method
hf	57.06	kJ/mol	Joback Method
hfus	10.80	kJ/mol	Joback Method
hvap	40.31	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.721		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	1120.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1147.10		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1147.10		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1150.00		NIST Webbook
ripol	1338.00		NIST Webbook

ripol	1338.00		NIST Webbook
ripol	1338.00		NIST Webbook
tb	481.48	K	Joback Method
tc	696.51	K	Joback Method
tf	235.32	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.48	J/mol×K	481.48	Joback Method
cpg	362.27	J/mol×K	517.32	Joback Method
cpg	380.72	J/mol×K	553.16	Joback Method
cpg	397.96	J/mol×K	588.99	Joback Method
cpg	414.11	J/mol×K	624.83	Joback Method
cpg	429.30	J/mol×K	660.67	Joback Method
cpg	443.64	J/mol×K	696.51	Joback Method
hvapt	47.80	kJ/mol	376.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6902734&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

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
hvapt: Enthalpy of vaporization at a given temperature

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