Isogeijerene

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/t11-,12-/
InchiKey: BGDQCKOAZKTOFV-RYUDHWBXSA-N
Formula: C12H18
SMILES: C=CC1(C)CCC=CC1C(=C)C
Mol. weight [g/mol]: 162.27

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
ripol	1304.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1304.00		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

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418363&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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