Isogeijerene C

Inchi: InChI=1S/C12H18/c1-5-12(4)9-7-6-8-11(12)10(2)3/h5-6,8H,1,7,9H2,2-4H3
InchiKey: DDDUDPZNWNWAHI-UHFFFAOYSA-N
Formula: C12H18
SMILES: C=CC1(C)CCC=CC1=C(C)C
Mol. weight [g/mol]: 162.27
CAS: 106494-41-1

Physical Properties

Property code	Value	Unit	Source
gf	223.83	kJ/mol	Joback Method
hf	28.00	kJ/mol	Joback Method
hfus	11.33	kJ/mol	Joback Method
hvap	42.07	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.865		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
ripol	1490.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1493.00		NIST Webbook
tb	496.11	K	Joback Method
tc	714.11	K	Joback Method
tf	251.68	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.69	J/mol×K	496.11	Joback Method
cpg	363.35	J/mol×K	532.44	Joback Method
cpg	380.74	J/mol×K	568.78	Joback Method
cpg	396.98	J/mol×K	605.11	Joback Method
cpg	412.22	J/mol×K	641.44	Joback Method
cpg	426.58	J/mol×K	677.78	Joback Method

cpg	440.20	J/mol×K	714.11	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=C106494411&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume