Brasila-1(6),5(10)-diene

Inchi: InChI=1S/C14H22/c1-9(2)13-7-10(3)8-14-11(4)5-6-12(13)14/h10-11H,5-8H2,1-4H3/t10-,
InchiKey: QAXOTPHOTITIST-MNOVXSKESA-N
Formula: C14H22
SMILES: CC(C)=C1CC(C)CC2=C1CCC2C
Mol. weight [g/mol]: 190.32

Physical Properties

Property code	Value	Unit	Source
gf	199.81	kJ/mol	Joback Method
hf	-104.09	kJ/mol	Joback Method
hfus	21.44	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.479		Crippen Method
mcvol	177.800	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
ripol	1529.00		NIST Webbook
tb	561.65	K	Joback Method
tc	777.37	K	Joback Method
tf	295.06	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.72	J/mol×K	561.65	Joback Method
cpg	470.47	J/mol×K	597.60	Joback Method
cpg	490.01	J/mol×K	633.56	Joback Method
cpg	508.41	J/mol×K	669.51	Joback Method
cpg	525.73	J/mol×K	705.47	Joback Method
cpg	542.03	J/mol×K	741.42	Joback Method
cpg	557.37	J/mol×K	777.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R337110&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
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