(5S,7S,10R)-cis-«beta»-Elemene, diastereomer

Inchi: InChI=1S/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,13-14H,1-2,4,8-10H2,3,5
InchiKey: OPFTUNCRGUEPRZ-RBSFLKMASA-N
Formula: C15H24
SMILES: C=CC1(C)CCC(C(=C)C)CC1C(=C)C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	325.38	kJ/mol	Joback Method
hf	32.66	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	45.79	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.747		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1387.00		NIST Webbook
rinpol	1387.00		NIST Webbook
tb	542.85	K	Joback Method
tc	754.13	K	Joback Method
tf	248.41	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.78	J/mol×K	542.85	Joback Method
cpg	511.42	J/mol×K	578.06	Joback Method
cpg	532.71	J/mol×K	613.28	Joback Method
cpg	552.77	J/mol×K	648.49	Joback Method
cpg	571.73	J/mol×K	683.70	Joback Method
cpg	589.70	J/mol×K	718.92	Joback Method
cpg	606.82	J/mol×K	754.13	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=R561729&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume