7«beta»H-Longifolane

Inchi: InChI=1S/C15H26/c1-10-11-6-7-12-13(11)14(2,3)8-5-9-15(10,12)4/h10-13H,5-9H2,1-4H3
InchiKey: OAYZLMHJYGEAAR-JHWMPXLRSA-N
Formula: C15H26
SMILES: CC1C2CCC3C2C(C)(C)CCCC13C
Mol. weight [g/mol]: 206.37

Physical Properties

Property code	Value	Unit	Source
gf	199.36	kJ/mol	Joback Method
hf	-177.39	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.495		Crippen Method
mcvol	189.630	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1467.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1633.00		NIST Webbook
tb	557.83	K	Joback Method
tc	780.06	K	Joback Method
tf	340.67	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.52	J/mol×K	557.83	Joback Method
cpg	547.59	J/mol×K	594.87	Joback Method
cpg	570.94	J/mol×K	631.91	Joback Method
cpg	592.86	J/mol×K	668.95	Joback Method
cpg	613.64	J/mol×K	705.99	Joback Method
cpg	633.54	J/mol×K	743.02	Joback Method

cpg	652.86	J/mol×K	780.06	Joback Method

Sources

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=R306473&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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