«beta»-Barbatene

Inchi: InChI=1S/C15H24/c1-11-6-9-13(2)10-12(11)14(3)7-5-8-15(13,14)4/h12H,1,5-10H2,2-4H3
InchiKey: RTONMYLSQISFQA-UHFFFAOYSA-N
Formula: C15H24
SMILES: C=C1CCC2(C)CC1C1(C)CCCC21C
Mol. weight [g/mol]: 204.35
CAS: 72346-55-5

Physical Properties

Property code	Value	Unit	Source
gf	262.37	kJ/mol	Joback Method
hf	-37.23	kJ/mol	Joback Method
hfus	5.83	kJ/mol	Joback Method
hvap	45.46	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1440.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1441.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1451.60		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1440.50		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1693.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1687.00		NIST Webbook

ripol	1689.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1693.00		NIST Webbook
ripol	1693.00		NIST Webbook
ripol	1693.00		NIST Webbook
ripol	1693.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1689.00		NIST Webbook
ripol	1693.00		NIST Webbook
tb	566.57	K	Joback Method
tc	800.20	K	Joback Method
tf	386.73	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.14	J/mol×K	566.57	Joback Method
cpg	522.76	J/mol×K	605.51	Joback Method
cpg	543.69	J/mol×K	644.45	Joback Method
cpg	563.39	J/mol×K	683.38	Joback Method
cpg	582.28	J/mol×K	722.32	Joback Method
cpg	600.82	J/mol×K	761.26	Joback Method
cpg	619.44	J/mol×K	800.20	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72346555&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

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