

«alpha»-Barbatene

Inchi: InChI=1S/C15H24/c1-11-6-9-13(2)10-12(11)14(3)7-5-8-15(13,14)4/h6,12H,5,7-10H2,1-4H
InchiKey: RMKQBFUAKZOV PQ-DKUMPPAJSA-N
Formula: C15H24
SMILES: CC1=CCC2(C)CC1C1(C)CCCC21C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	229.62	kJ/mol	Joback Method
hf	-75.16	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1416.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1432.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1627.50		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1623.00		NIST Webbook
tb	571.55	K	Joback Method
tc	806.48	K	Joback Method
tf	386.33	K	Joback Method
vc	0.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.53	J/mol×K	571.55	Joback Method
cpg	523.86	J/mol×K	610.71	Joback Method
cpg	544.56	J/mol×K	649.86	Joback Method
cpg	564.09	J/mol×K	689.02	Joback Method
cpg	582.88	J/mol×K	728.17	Joback Method
cpg	601.40	J/mol×K	767.33	Joback Method
cpg	620.08	J/mol×K	806.48	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=R127483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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

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