

bazzanene

Other names:	«beta»-Bazzanene
Inchi:	InChI=1S/C15H24/c1-12-7-10-14(3,11-8-12)15(4)9-5-6-13(15)2/h7H,2,5-6,8-11H2,1,3-4H
InchiKey:	YFLSTROSSKYYNK-HUUCEWRRSA-N
Formula:	C15H24
SMILES:	C=C1CCCC1(C)C1(C)CC=C(C)CC1
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	198.85	kJ/mol	Joback Method
hf	-77.10	kJ/mol	Joback Method
hfus	7.45	kJ/mol	Joback Method
hvap	48.48	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1519.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1519.00		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1789.50		NIST Webbook
ripol	1789.50		NIST Webbook
tb	581.21	K	Joback Method
tc	816.28	K	Joback Method
tf	351.85	K	Joback Method
vc	0.716	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.46	J/molxK	581.21	Joback Method
cpg	522.35	J/molxK	620.39	Joback Method

cpg	543.78	J/mol×K	659.57	Joback Method
cpg	564.03	J/mol×K	698.74	Joback Method
cpg	583.37	J/mol×K	737.92	Joback Method
cpg	602.08	J/mol×K	777.10	Joback Method
cpg	620.44	J/mol×K	816.28	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=R142011&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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