

(R)-3-Methylene-6-((S)-1,2,2-trimethylcyclopentyl)

Inchi:	InChI=1S/C15H24/c1-12-6-8-13(9-7-12)15(4)11-5-10-14(15,2)3/h6,8,13H,1,5,7,9-11H2,2
InchiKey:	QPXHUMFBJLASJO-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C1C=CC(C2(C)CCCC2(C)C)CC1
Mol. weight [g/mol]:	204.35
CAS:	98093-94-8

Physical Properties

Property code	Value	Unit	Source
gf	200.77	kJ/mol	Joback Method
hf	-85.97	kJ/mol	Joback Method
hfus	8.91	kJ/mol	Joback Method
hvap	47.51	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1546.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1550.90		NIST Webbook
tb	571.56	K	Joback Method
tc	805.60	K	Joback Method
tf	335.09	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.65	J/molxK	571.56	Joback Method
cpg	523.46	J/molxK	610.57	Joback Method
cpg	545.70	J/molxK	649.57	Joback Method
cpg	566.64	J/molxK	688.58	Joback Method
cpg	586.56	J/molxK	727.59	Joback Method
cpg	605.72	J/molxK	766.59	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=C98093948&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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