1,2,4-Methenoazulene, decahydro-1,5,5,8a-tetramethyl-, [1S-(1«alpha»,2«alpha»,3a«beta»,4«alpha»,8a«bet

Other names:	Longicyclene 1,2,4-Methenoazulene, decahydro-1,5,5,8a-tetramethyl-, [1S-(1«alpha»,2«alpha»,3a«beta»,4«alpha»,8a«beta»,9R)]- «alpha»-Longicyclene [1S-(1«alpha»,2«alpha»,3a«beta»,4«alpha»,8a«beta»,9R*)]-decahydro-1,5,5,8a-tetramet
Inchi:	InChI=1S/C15H24/c1-13(2)6-5-7-14(3)9-8-10-12(11(9)13)15(10,14)4/h9-12H,5-8H2,1-4H
InchiKey:	WCEIQUQVIOGRBF-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC1(C)CCCC2(C)C3CC4C(C31)C42C
Mol. weight [g/mol]:	204.35
CAS:	1137-12-8

Physical Properties

Property code	Value	Unit	Source
gf	290.92	kJ/mol	Joback Method
hf	-70.87	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	44.08	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	4.105		Crippen Method
mcvol	178.770	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1368.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1399.10		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1399.10		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1371.00		NIST Webbook

rinpol	1374.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1377.20		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1372.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1558.50		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1554.50		NIST Webbook
ripol	1558.50		NIST Webbook
ripol	1558.50		NIST Webbook
tb	552.00	K	Joback Method
tc	775.96	K	Joback Method
tf	393.07	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.97	J/mol×K	552.00	Joback Method
cpg	526.89	J/mol×K	589.33	Joback Method

cpg	547.94	J/mol×K	626.65	Joback Method
cpg	567.56	J/mol×K	663.98	Joback Method
cpg	586.20	J/mol×K	701.31	Joback Method
cpg	604.29	J/mol×K	738.63	Joback Method
cpg	622.26	J/mol×K	775.96	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=C1137128&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

Latest version available from:
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