Tricyclo[4.4.0.0(2,7)]decane, 1-methyl-3-methylene-8-(1-methylethyl)-, stereoisomer

Other names: Tricyclo[4.4.0.0(2,7)]decane, 8-isopropyl-1-methyl-3-methylene-, syn-8-
«beta»-Ylangene
trans-«beta»-Copaene
«beta»-Yalangene

Inchi: InChI=1S/C15H24/c1-9(2)11-7-8-15(4)12-6-5-10(3)14(15)13(11)12/h9,11-14H,3,5-8H2,1-

InchiKey: UPVZPMJSRSWJHQ-UHFFFAOYSA-N

Formula: C15H24

SMILES: C=C1CCC2C3C(C(C)C)CCC2(C)C13

Mol. weight [g/mol]: 204.35

CAS: 20479-06-5

Physical Properties

Property code	Value	Unit	Source
gf	275.30	kJ/mol	Joback Method
hf	-87.17	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	46.90	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1418.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1419.00		NIST Webbook

rinpol	1425.00	NIST Webbook
rinpol	1423.00	NIST Webbook
rinpol	1416.00	NIST Webbook
rinpol	1423.00	NIST Webbook
rinpol	1380.00	NIST Webbook
rinpol	1372.00	NIST Webbook
rinpol	1421.00	NIST Webbook
rinpol	1418.00	NIST Webbook
rinpol	1431.00	NIST Webbook
rinpol	1419.00	NIST Webbook
rinpol	1421.00	NIST Webbook
rinpol	1422.00	NIST Webbook
rinpol	1426.00	NIST Webbook
rinpol	1424.80	NIST Webbook
rinpol	1418.00	NIST Webbook
rinpol	1422.00	NIST Webbook
rinpol	1423.00	NIST Webbook
rinpol	1421.00	NIST Webbook
rinpol	1421.00	NIST Webbook
rinpol	1417.50	NIST Webbook
rinpol	1417.50	NIST Webbook
ripol	1586.00	NIST Webbook
ripol	1580.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1567.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1572.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1573.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1568.00	NIST Webbook
ripol	1576.00	NIST Webbook
ripol	1586.00	NIST Webbook
ripol	1589.00	NIST Webbook
ripol	1570.00	NIST Webbook
ripol	1553.00	NIST Webbook

ripol	1568.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1589.00		NIST Webbook
tb	556.71	K	Joback Method
tc	769.30	K	Joback Method
tf	323.21	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.63	J/mol×K	556.71	Joback Method
cpg	524.39	J/mol×K	592.14	Joback Method
cpg	545.67	J/mol×K	627.57	Joback Method
cpg	565.65	J/mol×K	663.00	Joback Method
cpg	584.49	J/mol×K	698.44	Joback Method
cpg	602.37	J/mol×K	733.87	Joback Method
cpg	619.46	J/mol×K	769.30	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20479065&Units=SI

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