Spiro[4.5]dec-7-ene, 1,8-dimethyl-4-(1-methylethenyl)-, [1S-(1«alpha»,4«beta»,5«alpha»)]-

Other names: Spiro[4.5]dec-7-ene, 1-isopropenyl-4,8-dimethyl-, [1S,4R,5S)-(-)-
Acoradien
Acoradiene

Inchi: InChI=1S/C15H24/c1-11(2)14-6-5-13(4)15(14)9-7-12(3)8-10-15/h7,13-14H,1,5-6,8-10H2

InchiKey: DVBSKQAFCDJNSL-UHFFFAOYSA-N

Formula: C15H24

SMILES: C=C(C)C1CCC(C)C12CC=C(C)CC2

Mol. weight [g/mol]: 204.35

CAS: 24048-44-0

Physical Properties

Property code	Value	Unit	Source
gf	234.94	kJ/mol	Joback Method
hf	-75.12	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1476.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1459.00		NIST Webbook
ripol	1698.00		NIST Webbook
ripol	1689.00		NIST Webbook
tb	569.43	K	Joback Method
tc	794.31	K	Joback Method

tf	297.83	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.65	J/mol×K	569.43	Joback Method
cpg	523.17	J/mol×K	606.91	Joback Method
cpg	545.19	J/mol×K	644.39	Joback Method
cpg	565.88	J/mol×K	681.87	Joback Method
cpg	585.40	J/mol×K	719.35	Joback Method
cpg	603.90	J/mol×K	756.83	Joback Method
cpg	621.57	J/mol×K	794.31	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=C24048440&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