

«alpha»-Dehydro-ar-himachalene

Inchi:	InChI=1S/C15H20/c1-11-7-8-13-12(2)6-5-9-15(3,4)14(13)10-11/h7-8,10H,2,5-6,9H2,1,3-
InchiKey:	LLYOXWSLVUQJHF-UHFFFAOYSA-N
Formula:	C15H20
SMILES:	C=C1CCCC(C)(C)c2cc(C)ccc21
Mol. weight [g/mol]:	200.32
CAS:	78204-62-3

Physical Properties

Property code	Value	Unit	Source
gf	252.71	kJ/mol	Joback Method
hf	20.62	kJ/mol	Joback Method
hfus	14.35	kJ/mol	Joback Method
hvap	51.85	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.470		Crippen Method
mcvol	183.290	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1522.60		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1517.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1882.00		NIST Webbook
tb	593.92	K	Joback Method
tc	826.15	K	Joback Method
tf	358.75	K	Joback Method
vc	0.691	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.85	J/mol×K	593.92	Joback Method

cpg	479.39	J/mol×K	632.63	Joback Method
cpg	497.74	J/mol×K	671.33	Joback Method
cpg	515.04	J/mol×K	710.04	Joback Method
cpg	531.45	J/mol×K	748.74	Joback Method
cpg	547.14	J/mol×K	787.45	Joback Method
cpg	562.25	J/mol×K	826.15	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=C78204623&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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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