

ar-Himachalene

Inchi:	InChI=1S/C15H22/c1-11-7-8-13-12(2)6-5-9-15(3,4)14(13)10-11/h7-8,10,12H,5-6,9H2,1-4
InchiKey:	RIHWULAZACSXEV-UHFFFAOYSA-N
Formula:	C15H22
SMILES:	<chem>Cc1ccc2c(c1)C(C)(C)CCCC2C</chem>
Mol. weight [g/mol]:	202.34
CAS:	19419-67-1

Physical Properties

Property code	Value	Unit	Source
gf	191.92	kJ/mol	Joback Method
hf	-83.96	kJ/mol	Joback Method
hfus	16.58	kJ/mol	Joback Method
hvap	51.38	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.560		Crippen Method
mvol	187.590	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	1541.90		NIST Webbook
tb	590.09	K	Joback Method
tc	820.32	K	Joback Method
tf	340.83	K	Joback Method
vc	0.706	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.51	J/mol×K	590.09	Joback Method
cpg	503.81	J/mol×K	628.46	Joback Method
cpg	523.82	J/mol×K	666.83	Joback Method
cpg	542.68	J/mol×K	705.21	Joback Method
cpg	560.55	J/mol×K	743.58	Joback Method
cpg	577.58	J/mol×K	781.95	Joback Method
cpg	593.92	J/mol×K	820.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19419671&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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