

(+)-isozierene

Inchi:	InChI=1S/C15H22/c1-12-5-3-4-6-13(2)15-10-9-14(11-15)8-7-12/h5,11,15H,2-4,6-10H2,1
InchiKey:	UTURGVPJEGEHFH-FDYAIDJWSA-N
Formula:	C15H22
SMILES:	C=C1CCCC=C(C)CCC2=CC1CC2
Mol. weight [g/mol]:	202.34

Physical Properties

Property code	Value	Unit	Source
gf	213.67	kJ/mol	Joback Method
hf	-53.25	kJ/mol	Joback Method
hfus	15.61	kJ/mol	Joback Method
hvap	52.39	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.789		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rmpol	1553.00		NIST Webbook
tb	598.08	K	Joback Method
tc	833.91	K	Joback Method
tf	314.53	K	Joback Method
vc	0.691	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.73	J/molxK	598.08	Joback Method
cpg	509.06	J/molxK	637.38	Joback Method
cpg	530.87	J/molxK	676.69	Joback Method
cpg	551.20	J/molxK	715.99	Joback Method
cpg	570.08	J/molxK	755.30	Joback Method
cpg	587.57	J/molxK	794.60	Joback Method
cpg	603.71	J/molxK	833.91	Joback Method
dvisc	0.0029120	Paxs	314.53	Joback Method
dvisc	0.0012764	Paxs	361.79	Joback Method

dvisc	0.0006770	Paxs	409.05	Joback Method
dvisc	0.0004094	Paxs	456.30	Joback Method
dvisc	0.0002721	Paxs	503.56	Joback Method
dvisc	0.0001940	Paxs	550.82	Joback Method
dvisc	0.0001459	Paxs	598.08	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=R406429&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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