

(-)-«beta»-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-ILXRZTDVSA-N
Formula:	C15H24
SMILES:	C=C(C)C1CCC(C)C12CC=C(C)CC2
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
hfus	15.49	kJ/mol	Joback Method
hvap	63.14	kJ/mol	Cheméo Relay (1.0)
ie	8.33	eV	Cheméo Relay (1.0)
log10ws	-5.13		Cheméo Relay (1.0)
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1468.00		NIST Webbook
rinpol	1468.00		NIST Webbook
tb	535.66	K	Cheméo Relay (1.0)
tf	242.61	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519921&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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