

«tau»-Elemene

Inchi:	InChI=1S/C15H24/c1-7-15(6)9-8-13(11(2)3)10-14(15)12(4)5/h7,13-14H,1-2,4,8-10H2,3,5
InchiKey:	OPFTUNCRGUEPRZ-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=CC1(C)CCC(C(=C)C)CC1C(=C)C
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
hfus	15.82	kJ/mol	Joback Method
logp	4.747		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
rinpol	1484.00		NIST Webbook
rinpol	1484.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.78	J/mol×K	542.85	Joback Method
cpg	511.42	J/mol×K	578.06	Joback Method
cpg	532.71	J/mol×K	613.28	Joback Method
cpg	552.77	J/mol×K	648.49	Joback Method
cpg	571.73	J/mol×K	683.70	Joback Method
cpg	589.70	J/mol×K	718.92	Joback Method
cpg	606.82	J/mol×K	754.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613206&Units=SI
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):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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