

«delta»-Cuprenene

Inchi:	InChI=1S/C15H24/c1-12-6-8-13(9-7-12)15(4)11-5-10-14(15,2)3/h6,8,13H,1,5,7,9-11H2,2
InchiKey:	QPXHUMFBJLASJO-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	<chem>C=C1C=CC(C2(C)CCCC2(C)C)CC1</chem>
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
hfus	8.91	kJ/mol	Joback Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1567.00		NIST Webbook
rinpol	1567.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1833.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.65	J/mol×K	571.56	Joback Method
cpg	523.46	J/mol×K	610.57	Joback Method
cpg	545.70	J/mol×K	649.57	Joback Method
cpg	566.64	J/mol×K	688.58	Joback Method
cpg	586.56	J/mol×K	727.59	Joback Method
cpg	605.72	J/mol×K	766.59	Joback Method
cpg	624.40	J/mol×K	805.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R338915&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
ripol: Polar retention indices

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