

ent-«alpha»-selinene

Inchi:	InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h6,13-14H,1,5,7-10H2,2
InchiKey:	OZQAPQSEYFAMCY-ZHDDOTHNSA-N
Formula:	C15H24
SMILES:	C=C(C)C1CCC2(C)CCC=C(C)C2C1
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
hfus	15.49	kJ/mol	Joback Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1554.70		NIST Webbook
rinpol	1560.00		NIST Webbook
ripol	1767.00		NIST Webbook
ripol	1765.40		NIST Webbook

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

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=R142180&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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