

«delta»-Selinene

Inchi:	InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h10-11H,5-9H2,1-4H3
InchiKey:	VEGYMPQCXPVQJY-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC1=C2C=C(C(C)C)CCC2(C)CCC1
Mol. weight [g/mol]:	204.35
CAS:	28624-28-4

Physical Properties

Property code	Value	Unit	Source
gf	179.33	kJ/mol	Joback Method
hf	-120.52	kJ/mol	Joback Method
hfus	12.86	kJ/mol	Joback Method
hvap	50.84	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mvol	191.890	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1496.90		NIST Webbook
tb	590.89	K	Joback Method
tc	815.98	K	Joback Method
tf	332.83	K	Joback Method
vc	0.723	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.51	J/molxK	590.89	Joback Method
cpg	521.85	J/molxK	628.41	Joback Method
cpg	541.90	J/molxK	665.92	Joback Method
cpg	560.83	J/molxK	703.44	Joback Method
cpg	578.78	J/molxK	740.95	Joback Method
cpg	595.93	J/molxK	778.47	Joback Method
cpg	612.42	J/molxK	815.98	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=C28624284&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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