

Isospathulenol

Inchi:	InChI=1S/C15H24O/c1-9-5-6-11-13(14(11,2)3)12-10(9)7-8-15(12,4)16/h10-13,16H,1,5-8
InchiKey:	FRMCCTDTYSRUBE-KMCWBVRRSA-N
Formula:	C15H24O
SMILES:	C=C1CCC2C(C3C1CCC3(C)O)C2(C)C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
hfus	18.36	kJ/mol	Joback Method
logp	3.386		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
tb	556.73	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.53	J/mol×K	649.17	Joback Method
cpg	594.60	J/mol×K	683.79	Joback Method
cpg	612.82	J/mol×K	718.40	Joback Method
cpg	630.40	J/mol×K	753.02	Joback Method
cpg	647.59	J/mol×K	787.63	Joback Method
cpg	664.58	J/mol×K	822.25	Joback Method
cpg	681.62	J/mol×K	856.86	Joback Method

Sources

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=R610509&Units=SI>

Joback Method:

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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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