

geranyl-p-cymene

Inchi:	InChI=1S/C20H30/c1-16(2)8-6-9-17(3)10-7-11-19(5)20-14-12-18(4)13-15-20/h8,10,12-15
InchiKey:	IKVVTAAICQTCAL-XNTDXEJSSA-N
Formula:	C20H30
SMILES:	<chem>CC(C)=CCC/C(C)=C/CCC(C)c1ccc(C)cc1</chem>
Mol. weight [g/mol]:	270.46

Physical Properties

Property code	Value	Unit	Source
hfus	35.47	kJ/mol	Joback Method
log10ws	-6.75		Cheméo Relay (1.0)
logp	6.571		Crippen Method
mcvol	260.300	ml/mol	McGowan Method
tb	601.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.01	J/mol×K	696.30	Joback Method
cpg	743.14	J/mol×K	730.39	Joback Method
cpg	762.12	J/mol×K	764.48	Joback Method
cpg	780.05	J/mol×K	798.56	Joback Method
cpg	796.99	J/mol×K	832.65	Joback Method
cpg	813.01	J/mol×K	866.74	Joback Method
cpg	828.21	J/mol×K	900.83	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55968439&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):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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