(Z)-«beta»-Terpinolene

Inchi: InChI=1S/C10H16/c1-8(2)10-6-4-9(3)5-7-10/h4H,5-7H2,1-3H3
InchiKey: MOYAFQVGZZPNRA-UHFFFAOYSA-N
Formula: C10H16
SMILES: CC1=CCC(=C(C)C)CC1
Mol. weight [g/mol]: 136.23

Physical Properties

Property code	Value	Unit	Source
hfus	12.27	kJ/mol	Joback Method
logp	3.453		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.08	J/mol×K	463.08	Joback Method
cpg	288.73	J/mol×K	498.41	Joback Method
cpg	304.49	J/mol×K	533.74	Joback Method
cpg	319.40	J/mol×K	569.07	Joback Method
cpg	333.48	J/mol×K	604.40	Joback Method
cpg	346.77	J/mol×K	639.73	Joback Method
cpg	359.30	J/mol×K	675.06	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R616225&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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices