«alpha»-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	1100.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1104.00		NIST Webbook
ripol	1278.00		NIST Webbook
ripol	1278.00		NIST Webbook
ripol	1288.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R606872&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):	
Cheméo Relay (1.0, beta):	

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