

2,2,9,9-TETRAMETHYLDEC-5-ENE-3,7-DIYNE

Inchi:	InChI=1S/C14H20/c1-13(2,3)11-9-7-8-10-12-14(4,5)6/h7-8H,1-6H3/b8-7-
InchiKey:	UUSGALMHPVDLPR-BQYQJAHWSA-N
Formula:	C14H20
SMILES:	CC(C)(C)C#C/C=C/C#CC(C)(C)C
Mol. weight [g/mol]:	188.31

Physical Properties

Property code	Value	Unit	Source
hfus	23.63	kJ/mol	Joback Method
ie	8.46	eV	Cheméo Relay (1.0)
logp	3.642		Crippen Method
mcvol	186.620	ml/mol	McGowan Method
tb	472.46	K	Cheméo Relay (1.0)
tf	371.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.91	J/mol×K	535.42	Joback Method
cpg	446.54	J/mol×K	574.80	Joback Method
cpg	464.76	J/mol×K	614.18	Joback Method
cpg	481.68	J/mol×K	653.56	Joback Method
cpg	497.41	J/mol×K	692.94	Joback Method
cpg	512.05	J/mol×K	732.32	Joback Method
cpg	525.74	J/mol×K	771.70	Joback Method

Sources

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):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C102745357&Units=SI>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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