

Tricyclo[4.2.0.0^{2,5}]octane,1,2,5,6-tetramethyl-3,4,7-trimethyl-

Other names:	Tricyclo[4.2.0.0
Inchi:	InChI=1S/C16H20/c1-9-10(2)14(6)13(9,5)15(7)11(3)12(4)16(14,15)8/h1-4H2,5-8H3
InchiKey:	RRNQSOQWCKWZLJ-UHFFFAOYSA-N
Formula:	C16H20
SMILES:	C=C1C(=C)C2(C)C1(C)C1(C)C(=C)C(=C)C21C
Mol. weight [g/mol]:	212.34

Physical Properties

Property code	Value	Unit	Source
hfus	4.94	kJ/mol	Joback Method
ie	8.10 ± 0.02	eV	NIST Webbook
logp	4.277		Crippen Method
mcvol	186.520	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.52	J/mol×K	574.36	Joback Method
cpg	499.42	J/mol×K	611.11	Joback Method
cpg	514.21	J/mol×K	647.85	Joback Method
cpg	528.36	J/mol×K	684.60	Joback Method
cpg	542.33	J/mol×K	721.34	Joback Method
cpg	556.59	J/mol×K	758.09	Joback Method
cpg	571.59	J/mol×K	794.83	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C34101241&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

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

Latest version available from:

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