

2,4,4-Trimethylcyclopentanone

Other names:	2,4,4-Trimethylcyclopentanone 2,4,4-trimethylcyclopentan-1-one
Inchi:	InChI=1S/C8H14O/c1-6-4-8(2,3)5-7(6)9/h6H,4-5H2,1-3H3
InchiKey:	OXTQEWUBDTVSFB-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CC1CC(C)(C)CC1=O
Mol. weight [g/mol]:	126.20

Physical Properties

Property code	Value	Unit	Source
hfus	4.69	kJ/mol	Joback Method
ie	9.30	eV	Cheméo Relay (1.0)
logp	2.012		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
tb	428.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.57	J/mol×K	461.11	Joback Method
cpg	265.00	J/mol×K	497.96	Joback Method
cpg	280.47	J/mol×K	534.82	Joback Method
cpg	295.06	J/mol×K	571.67	Joback Method
cpg	308.86	J/mol×K	608.53	Joback Method
cpg	321.95	J/mol×K	645.38	Joback Method
cpg	334.42	J/mol×K	682.24	Joback Method

Sources

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=C4694126&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>

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

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