2,2,4-Trimethylcyclopentanone

Other names: 2,2,4-Trimethylcyclopentanone
2,2,4-trimethylcyclopentan-1-one
Inchi: InChI=1S/C8H14O/c1-6-4-7(9)8(2,3)5-6/h6H,4-5H2,1-3H3
InchiKey: PJXIBUIXCXSNCM-UHFFFAOYSA-N
Formula: C8H14O
SMILES: CC1CC(=O)C(C)(C)C1
Mol. weight [g/mol]: 126.20

Physical Properties

Property code	Value	Unit	Source
hfus	4.69	kJ/mol	Joback Method
logp	2.012		Crippen Method
mcvol	114.290	ml/mol	McGowan Method

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

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=C28056544&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume