2,5,6-Trimethyl-2-cyclohexen-1-one

Other names: 2,5,6-Trimethyl-2-cyclohexen-1-one
Inchi: InChI=1S/C9H14O/c1-6-4-5-7(2)9(10)8(6)3/h5-6,8H,4H2,1-3H3
InchiKey: QAQCUBLNHBKTRM-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC1=CCC(C)C(C)C1=O
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
hfus	12.31	kJ/mol	Joback Method
logp	2.178		Crippen Method
mcvol	124.080	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.29	J/mol×K	492.16	Joback Method
cpg	293.01	J/mol×K	528.87	Joback Method
cpg	309.03	J/mol×K	565.57	Joback Method
cpg	324.34	J/mol×K	602.28	Joback Method
cpg	338.93	J/mol×K	638.98	Joback Method
cpg	352.77	J/mol×K	675.69	Joback Method
cpg	365.86	J/mol×K	712.40	Joback Method
cpl	258.40	J/mol×K	298.15	NIST Webbook
cpl	258.10	J/mol×K	298.15	NIST Webbook
hvapt	45.50 ± 0.30	kJ/mol	424.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20030302&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):	

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume