2,5,6-trimethylcyclohex-2-en-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
CAS: 20030-30-2

Physical Properties

Property code	Value	Unit	Source
gf	-60.62	kJ/mol	Joback Method
hf	-286.50	kJ/mol	Joback Method
hfus	12.31	kJ/mol	Joback Method
hvap	40.95	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.178		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	492.16	K	Joback Method
tc	712.40	K	Joback Method
tf	275.83	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.77	J/mol×K	675.69	Joback Method
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	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20030302&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume