2-Cyclohexen-1-one, 3,4,4-trimethyl-

Inchi: InChI=1S/C9H14O/c1-7-6-8(10)4-5-9(7,2)3/h6H,4-5H2,1-3H3
InchiKey: LJILDAULEWAKOE-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC1=CC(=O)CCC1(C)C
Mol. weight [g/mol]: 138.21
CAS: 17299-41-1

Physical Properties

Property code	Value	Unit	Source
gf	-58.40	kJ/mol	Joback Method
hf	-250.92	kJ/mol	Joback Method
hfus	4.95	kJ/mol	Joback Method
hvap	40.11	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1198.00		NIST Webbook
ripol	1720.00		NIST Webbook
tb	490.20	K	NIST Webbook
tc	727.23	K	Joback Method
tf	303.97	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.69	J/mol×K	497.07	Joback Method
cpg	291.98	J/mol×K	535.43	Joback Method
cpg	307.32	J/mol×K	573.79	Joback Method
cpg	321.80	J/mol×K	612.15	Joback Method
cpg	335.52	J/mol×K	650.51	Joback Method
cpg	348.57	J/mol×K	688.87	Joback Method
cpg	361.03	J/mol×K	727.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.20	K	1.70	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17299411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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