

2,5-Heptadien-4-one, 2,6-dimethyl-

Other names:	2,5-Heptadien-4-one, 2,6-dimethyl- 2,6-Dimethyl-2,5-heptadien-4-one 2,6-dimethylhepta-2,5-dien-4-one Diisobutenyl ketone Diisopropylidene acetone Foron NSC 38718 Phoron s-Diisopropylidene acetone sym-Diisopropylidene acetone
Inchi:	InChI=1S/C9H14O/c1-7(2)5-9(10)6-8(3)4/h5-6H,1-4H3
InchiKey:	MTZWHHIREPJPTG-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC(C)=CC(=O)C=C(C)C
Mol. weight [g/mol]:	138.21

Physical Properties

Property code	Value	Unit	Source
hf	-173.78	kJ/mol	Cheméo Relay (1.0)
hfus	18.45	kJ/mol	Joback Method
hvap	53.05	kJ/mol	Cheméo Relay (1.0)
ie	8.70	eV	Cheméo Relay (1.0)
logp	2.488		Crippen Method
mcvol	130.640	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1092.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1564.00		NIST Webbook
tb	470.70	K	NIST Webbook
tb	470.15 ± 2.00	K	NIST Webbook
tc	651.30	K	Cheméo Relay (1.0)
tf	299.00 ± 0.50	K	NIST Webbook
tf	301.15 ± 2.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.84	J/mol×K	467.27	Joback Method
cpg	278.12	J/mol×K	500.34	Joback Method
cpg	290.66	J/mol×K	533.40	Joback Method
cpg	302.48	J/mol×K	566.47	Joback Method
cpg	313.64	J/mol×K	599.54	Joback Method
cpg	324.18	J/mol×K	632.60	Joback Method
cpg	334.13	J/mol×K	665.67	Joback Method
hvapt	54.10	kJ/mol	393.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C504201&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

Legend

cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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

tc: Critical Temperature
tf: Normal melting (fusion) point

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