4,4-DIMETHYL-2-PENTYNAL

Other names: 4,4-Dimethyl-2-pentynal
Inchi: InChI=1S/C7H10O/c1-7(2,3)5-4-6-8/h6H,1-3H3
InchiKey: DTMPOWDLMOYPDD-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CC(C)(C)C#CC=O
Mol. weight [g/mol]: 110.16

Physical Properties

Property code	Value	Unit	Source
hfus	11.88	kJ/mol	Joback Method
ie	10.03	eV	NIST Webbook
logp	1.235		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
tb	414.63	K	Cheméo Relay (1.0)
tf	278.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.36	J/mol×K	413.99	Joback Method
cpg	203.42	J/mol×K	448.99	Joback Method
cpg	213.83	J/mol×K	483.99	Joback Method
cpg	223.62	J/mol×K	518.99	Joback Method
cpg	232.82	J/mol×K	553.99	Joback Method
cpg	241.45	J/mol×K	588.99	Joback Method
cpg	249.56	J/mol×K	623.99	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=C2579217&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point