

6,10,14-pentadecanone

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H36O/c1-15(2)9-6-10-16(3)11-7-12-17(4)13-8-14-18(5)19/h15-17H,6-14H2

WHWDWIHXSPCOKZ-UHFFFAOYSA-N

C18H36O

CC(=O)CCCC(C)CCCC(C)CCCC(C)C

268.48

Physical Properties

Property code	Value	Unit	Source
gf	-35.56	kJ/mol	Joback Method
hf	-543.27	kJ/mol	Joback Method
hfus	33.41	kJ/mol	Joback Method
hvap	61.24	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	6.015		Crippen Method
mcvol	266.050	ml/mol	McGowan Method
pc	1223.41	kPa	Joback Method
rinpol	1834.00		NIST Webbook
rinpol	1834.00		NIST Webbook
tb	663.79	K	Joback Method
tc	837.19	K	Joback Method
tf	297.55	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.01	J/mol×K	663.79	Joback Method
cpg	849.23	J/mol×K	808.29	Joback Method
cpg	832.90	J/mol×K	779.39	Joback Method
cpg	815.74	J/mol×K	750.49	Joback Method
cpg	797.72	J/mol×K	721.59	Joback Method
cpg	778.82	J/mol×K	692.69	Joback Method
cpg	864.76	J/mol×K	837.19	Joback Method
dvisc	0.0000989	Pa×s	663.79	Joback Method

dvisc	0.0001419	Pa×s	602.75	Joback Method
dvisc	0.0002208	Pa×s	541.71	Joback Method
dvisc	0.0003843	Pa×s	480.67	Joback Method
dvisc	0.0007862	Pa×s	419.63	Joback Method
dvisc	0.0020519	Pa×s	358.59	Joback Method
dvisc	0.0079383	Pa×s	297.55	Joback Method

Sources

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=R340517&Units=SI
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
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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