2-Hexadecanone, 6,10,14-trimethyl

Inchi: InChI=1S/C19H38O/c1-6-16(2)10-7-11-17(3)12-8-13-18(4)14-9-15-19(5)20/h16-18H,6-15
InchiKey: SMCRXBLMFXFLRR-UHFFFAOYSA-N
Formula: C19H38O
SMILES: CCC(C)CCCC(C)CCCC(C)CCCC(C)=O
Mol. weight [g/mol]: 282.50

Physical Properties

Property code	Value	Unit	Source
gf	-27.14	kJ/mol	Joback Method
hf	-563.91	kJ/mol	Joback Method
hfus	36.00	kJ/mol	Joback Method
hvap	63.47	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	6.405		Crippen Method
mcvol	280.140	ml/mol	McGowan Method
pc	1145.21	kPa	Joback Method
rinpol	1953.00		NIST Webbook
tb	686.67	K	Joback Method
tc	860.10	K	Joback Method
tf	308.82	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.30	J/mol×K	686.67	Joback Method
cpg	908.90	J/mol×K	831.19	Joback Method
cpg	892.34	J/mol×K	802.29	Joback Method
cpg	874.93	J/mol×K	773.38	Joback Method
cpg	856.64	J/mol×K	744.48	Joback Method
cpg	837.44	J/mol×K	715.57	Joback Method
cpg	924.64	J/mol×K	860.10	Joback Method
dvisc	0.0000869	Pa×s	686.67	Joback Method
dvisc	0.0001247	Pa×s	623.69	Joback Method

dvisc	0.0001942	Pa×s	560.72	Joback Method
dvisc	0.0003382	Pa×s	497.75	Joback Method
dvisc	0.0006919	Pa×s	434.77	Joback Method
dvisc	0.0018034	Pa×s	371.79	Joback Method
dvisc	0.0069481	Pa×s	308.82	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=R556648&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