2-Dodecanone, 6,10-dimethyl

Inchi: InChI=1S/C14H28O/c1-5-12(2)8-6-9-13(3)10-7-11-14(4)15/h12-13H,5-11H2,1-4H3
InchiKey: CVUJPEFABHFRBO-UHFFFAOYSA-N
Formula: C14H28O
SMILES: CCC(C)CCCC(C)CCCC(C)=O
Mol. weight [g/mol]: 212.37

Physical Properties

Property code	Value	Unit	Source
gf	-66.80	kJ/mol	Joback Method
hf	-455.43	kJ/mol	Joback Method
hfus	26.57	kJ/mol	Joback Method
hvap	52.73	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.598		Crippen Method
mcvol	209.690	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	1500.00		NIST Webbook
tb	572.71	K	Joback Method
tc	746.61	K	Joback Method
tf	267.47	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.15	J/mol×K	572.71	Joback Method
cpg	619.86	J/mol×K	717.63	Joback Method
cpg	604.99	J/mol×K	688.65	Joback Method
cpg	589.40	J/mol×K	659.66	Joback Method
cpg	573.08	J/mol×K	630.68	Joback Method
cpg	556.00	J/mol×K	601.69	Joback Method
cpg	634.03	J/mol×K	746.61	Joback Method
dvisc	0.0001695	Pa×s	572.71	Joback Method
dvisc	0.0002362	Pa×s	521.84	Joback Method

dvisc	0.0003537	Pa×s	470.96	Joback Method
dvisc	0.0005840	Pa×s	420.09	Joback Method
dvisc	0.0011073	Pa×s	369.22	Joback Method
dvisc	0.0025759	Pa×s	318.34	Joback Method
dvisc	0.0082611	Pa×s	267.47	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=R556633&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