11-Methyl-2-tridecanone

Inchi: InChI=1S/C14H28O/c1-4-13(2)11-9-7-5-6-8-10-12-14(3)15/h13H,4-12H2,1-3H3
InchiKey: RGQOHKMKTPQXIW-UHFFFAOYSA-N
Formula: C14H28O
SMILES: CCC(C)CCCCCCCCC(C)=O
Mol. weight [g/mol]: 212.37

Physical Properties

Property code	Value	Unit	Source
gf	-64.36	kJ/mol	Joback Method
hf	-450.15	kJ/mol	Joback Method
hfus	30.09	kJ/mol	Joback Method
hvap	53.12	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.742		Crippen Method
mcvol	209.690	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	1573.00		NIST Webbook
tb	573.15	K	Joback Method
tc	744.08	K	Joback Method
tf	282.47	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.86	J/mol×K	573.15	Joback Method
cpg	618.10	J/mol×K	715.59	Joback Method
cpg	603.46	J/mol×K	687.10	Joback Method
cpg	588.14	J/mol×K	658.62	Joback Method
cpg	572.11	J/mol×K	630.13	Joback Method
cpg	555.36	J/mol×K	601.64	Joback Method
cpg	632.08	J/mol×K	744.08	Joback Method
dvisc	0.0001809	Pa×s	573.15	Joback Method
dvisc	0.0002462	Pa×s	524.70	Joback Method

dvisc	0.0003567	Pa×s	476.26	Joback Method
dvisc	0.0005621	Pa×s	427.81	Joback Method
dvisc	0.0009950	Pa×s	379.36	Joback Method
dvisc	0.0020815	Pa×s	330.92	Joback Method
dvisc	0.0056093	Pa×s	282.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R412563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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