

2,12-Dimethyltridecan-4-one

Inchi:	InChI=1S/C15H30O/c1-13(2)10-8-6-5-7-9-11-15(16)12-14(3)4/h13-14H,5-12H2,1-4H3
InchiKey:	RGMWWSCJNNLNK-UHFFFAOYSA-N
Formula:	C15H30O
SMILES:	CC(C)CCCCCCCC(=O)CC(C)C
Mol. weight [g/mol]:	226.40

Physical Properties

Property code	Value	Unit	Source
gf	-58.38	kJ/mol	Joback Method
hf	-476.07	kJ/mol	Joback Method
hfus	29.16	kJ/mol	Joback Method
hvap	54.95	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.988		Crippen Method
mcvol	223.780	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	1589.00		NIST Webbook
tb	595.59	K	Joback Method
tc	768.36	K	Joback Method
tf	278.74	K	Joback Method
vc	0.870	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.20	J/mol×K	595.59	Joback Method
cpg	675.06	J/mol×K	739.56	Joback Method
cpg	659.80	J/mol×K	710.77	Joback Method
cpg	643.82	J/mol×K	681.97	Joback Method
cpg	627.07	J/mol×K	653.18	Joback Method
cpg	609.53	J/mol×K	624.38	Joback Method
cpg	689.59	J/mol×K	768.36	Joback Method
dvisc	0.0001521	Paxs	595.59	Joback Method
dvisc	0.0002125	Paxs	542.78	Joback Method

dvisc	0.0003189	Paxs	489.97	Joback Method
dvisc	0.0005279	Paxs	437.17	Joback Method
dvisc	0.0010038	Paxs	384.36	Joback Method
dvisc	0.0023422	Paxs	331.55	Joback Method
dvisc	0.0075344	Paxs	278.74	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R508822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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