

9-Methyl-1-phenyldecan-1-one

Inchi:	InChI=1S/C17H26O/c1-15(2)11-7-4-3-5-10-14-17(18)16-12-8-6-9-13-16/h6,8-9,12-13,15
InchiKey:	NWMOWTHLIXLVOY-UHFFFAOYSA-N
Formula:	C17H26O
SMILES:	CC(C)CCCCCCC(=O)c1ccccc1
Mol. weight [g/mol]:	246.39

Physical Properties

Property code	Value	Unit	Source
gf	73.31	kJ/mol	Joback Method
hf	-275.54	kJ/mol	Joback Method
hfus	31.90	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.256		Crippen Method
mcvol	228.200	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	1966.00		NIST Webbook
rinpol	1966.00		NIST Webbook
tb	668.47	K	Joback Method
tc	866.19	K	Joback Method
tf	342.70	K	Joback Method
vc	0.879	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.06	J/mol×K	668.47	Joback Method
cpg	644.30	J/mol×K	701.42	Joback Method
cpg	661.50	J/mol×K	734.38	Joback Method
cpg	677.69	J/mol×K	767.33	Joback Method
cpg	692.93	J/mol×K	800.28	Joback Method
cpg	707.26	J/mol×K	833.24	Joback Method
cpg	720.73	J/mol×K	866.19	Joback Method
dvisc	0.0030763	Paxs	342.70	Joback Method

dvisc	0.0012641	Paxs	397.00	Joback Method
dvisc	0.0006434	Paxs	451.29	Joback Method
dvisc	0.0003786	Paxs	505.59	Joback Method
dvisc	0.0002469	Paxs	559.88	Joback Method
dvisc	0.0001736	Paxs	614.17	Joback Method
dvisc	0.0001293	Paxs	668.47	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=R508897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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