

3-Methyltridecan-4-one

Inchi:	InChI=1S/C14H28O/c1-4-6-7-8-9-10-11-12-14(15)13(3)5-2/h13H,4-12H2,1-3H3
InchiKey:	MTDKYNCGFZGFIY-UHFFFAOYSA-N
Formula:	C14H28O
SMILES:	CCCCCCCCC(=O)C(C)CC
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	1532.00		NIST Webbook
rinpol	1532.00		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/molxK	573.15	Joback Method
cpg	555.36	J/molxK	601.64	Joback Method
cpg	572.11	J/molxK	630.13	Joback Method
cpg	588.14	J/molxK	658.62	Joback Method
cpg	603.46	J/molxK	687.10	Joback Method
cpg	618.10	J/molxK	715.59	Joback Method
cpg	632.08	J/molxK	744.08	Joback Method
dvisc	0.0056093	Paxs	282.47	Joback Method

dvisc	0.0020815	Paxs	330.92	Joback Method
dvisc	0.0009950	Paxs	379.36	Joback Method
dvisc	0.0005621	Paxs	427.81	Joback Method
dvisc	0.0003567	Paxs	476.26	Joback Method
dvisc	0.0002462	Paxs	524.70	Joback Method
dvisc	0.0001809	Paxs	573.15	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=R508862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log_p:	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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