

(Z)-6-Pentadecen-2-one

Inchi:	InChI=1S/C15H28O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15(2)16/h10-11H,3-9,12-14H2,1-2H
InchiKey:	BDLYSBLBXYIRW-KHPPLWFESA-N
Formula:	C15H28O
SMILES:	CCCCCCCCC=CCCC(C)=O
Mol. weight [g/mol]:	224.38

Physical Properties

Property code	Value	Unit	Source
gf	26.72	kJ/mol	Joback Method
hf	-348.29	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	55.69	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	5.053		Crippen Method
mcvol	219.480	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook
tb	600.63	K	Joback Method
tc	773.80	K	Joback Method
tf	303.66	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.12	J/mol×K	600.63	Joback Method
cpg	650.14	J/mol×K	744.94	Joback Method
cpg	635.78	J/mol×K	716.08	Joback Method
cpg	620.73	J/mol×K	687.22	Joback Method
cpg	604.95	J/mol×K	658.35	Joback Method
cpg	588.42	J/mol×K	629.49	Joback Method

cpg	663.84	J/mol×K	773.80	Joback Method
dvisc	0.0001489	Pa×s	600.63	Joback Method
dvisc	0.0001992	Pa×s	551.13	Joback Method
dvisc	0.0002822	Pa×s	501.64	Joback Method
dvisc	0.0004315	Pa×s	452.14	Joback Method
dvisc	0.0007322	Pa×s	402.65	Joback Method
dvisc	0.0014411	Pa×s	353.15	Joback Method
dvisc	0.0035368	Pa×s	303.66	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R420465&Units=SI

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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