

3-Pentadecen-2-one, 6,10,14-trimethyl

Inchi:	InChI=1S/C18H34O/c1-15(2)9-6-10-16(3)11-7-12-17(4)13-8-14-18(5)19/h8,14-17H,6-7,9
InchiKey:	UDQNYFAGVRXQCM-RIYZIHGNSA-N
Formula:	C18H34O
SMILES:	CC(=O)C=CCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]:	266.46

Physical Properties

Property code	Value	Unit	Source
gf	44.66	kJ/mol	Joback Method
hf	-426.05	kJ/mol	Joback Method
hfus	33.61	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.791		Crippen Method
mcvol	261.750	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	1877.00		NIST Webbook
rinpol	1877.00		NIST Webbook
tb	667.95	K	Joback Method
tc	846.56	K	Joback Method
tf	292.47	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.83	J/molxK	667.95	Joback Method
cpg	757.25	J/molxK	697.72	Joback Method
cpg	775.74	J/molxK	727.49	Joback Method
cpg	793.32	J/molxK	757.25	Joback Method
cpg	810.05	J/molxK	787.02	Joback Method
cpg	825.95	J/molxK	816.79	Joback Method
cpg	841.07	J/molxK	846.56	Joback Method
dvisc	0.0076520	Paxs	292.47	Joback Method

dvisc	0.0018665	Paxs	355.05	Joback Method
dvisc	0.0006949	Paxs	417.63	Joback Method
dvisc	0.0003347	Paxs	480.21	Joback Method
dvisc	0.0001908	Paxs	542.79	Joback Method
dvisc	0.0001221	Paxs	605.37	Joback Method
dvisc	0.0000850	Paxs	667.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R194171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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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