

8,11,14-heptadecatrien-2-one

Inchi:	InChI=1S/C17H28O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(2)18/h4-5,7-8,10-11H,3,6
InchiKey:	QBIODMBDIAZVIW-JSIPCRQOSA-N
Formula:	C17H28O
SMILES:	CCC=CCC=CCC=CCCCCCC(C)=O
Mol. weight [g/mol]:	248.40

Physical Properties

Property code	Value	Unit	Source
gf	204.00	kJ/mol	Joback Method
hf	-155.13	kJ/mol	Joback Method
hfus	41.99	kJ/mol	Joback Method
hvap	60.06	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.385		Crippen Method
mcvol	239.060	ml/mol	McGowan Method
pc	1444.64	kPa	Joback Method
ripol	2611.00		NIST Webbook
ripol	2611.00		NIST Webbook
tb	654.71	K	Joback Method
tc	837.68	K	Joback Method
tf	316.04	K	Joback Method
vc	0.933	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.11	J/mol×K	654.71	Joback Method
cpg	655.45	J/mol×K	685.21	Joback Method
cpg	671.92	J/mol×K	715.70	Joback Method
cpg	687.57	J/mol×K	746.20	Joback Method
cpg	702.47	J/mol×K	776.69	Joback Method
cpg	716.66	J/mol×K	807.19	Joback Method
cpg	730.20	J/mol×K	837.68	Joback Method
dvisc	0.0026899	Paxs	316.04	Joback Method

dvisc	0.0009893	Paxs	372.48	Joback Method
dvisc	0.0004734	Paxs	428.93	Joback Method
dvisc	0.0002689	Paxs	485.38	Joback Method
dvisc	0.0001719	Paxs	541.82	Joback Method
dvisc	0.0001195	Paxs	598.27	Joback Method
dvisc	0.0000885	Paxs	654.71	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=R308177&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
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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