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	m3/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	Pa×s	316.04	Joback Method

dvisc	0.0009893	Pa×s	372.48	Joback Method
dvisc	0.0004734	Pa×s	428.93	Joback Method
dvisc	0.0002689	Pa×s	485.38	Joback Method
dvisc	0.0001719	Pa×s	541.82	Joback Method
dvisc	0.0001195	Pa×s	598.27	Joback Method
dvisc	0.0000885	Pa×s	654.71	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=R308177&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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