E-15-Heptadecenal

Inchi: InChI=1S/C17H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18/h2-3,17H,4-16H2,1
InchiKey: TWWSXAKLFHYWQT-NSCUHMNNSA-N
Formula: C17H32O
SMILES: CC=CCCCCCCCCCCCCCC=O
Mol. weight [g/mol]: 252.44

Physical Properties

Property code	Value	Unit	Source
gf	72.96	kJ/mol	Joback Method
hf	-362.57	kJ/mol	Joback Method
hfus	42.28	kJ/mol	Joback Method
hvap	60.11	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.833		Crippen Method
mcvol	247.660	ml/mol	McGowan Method
pc	1347.68	kPa	Joback Method
rinpol	2084.50		NIST Webbook
rinpol	2085.50		NIST Webbook
rinpol	2083.20		NIST Webbook
rinpol	2104.00		NIST Webbook
tb	641.18	K	Joback Method
tc	810.06	K	Joback Method
tf	318.27	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.41	J/mol×K	641.18	Joback Method
cpg	697.32	J/mol×K	669.33	Joback Method
cpg	714.44	J/mol×K	697.47	Joback Method
cpg	730.79	J/mol×K	725.62	Joback Method
cpg	746.41	J/mol×K	753.76	Joback Method
cpg	761.32	J/mol×K	781.91	Joback Method

cpg	775.57	J/mol×K	810.06	Joback Method
dvisc	0.0035586	Pa×s	318.27	Joback Method
dvisc	0.0013828	Pa×s	372.09	Joback Method
dvisc	0.0006823	Pa×s	425.91	Joback Method
dvisc	0.0003945	Pa×s	479.73	Joback Method
dvisc	0.0002547	Pa×s	533.54	Joback Method
dvisc	0.0001782	Pa×s	587.36	Joback Method
dvisc	0.0001324	Pa×s	641.18	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=U130979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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