

Z-2-TETRADECEN-1-OL ACETATE

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C16H30O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-16(2)17/h13-14H,3-12,15H

VUMJUHLCRBNTAR-YPKPFQOOSA-N

C16H30O2

CCCCCCCCCCC/C=C\COC(C)=O

254.41

Physical Properties

Property code	Value	Unit	Source
af	0.7421		Cheméo Relay (1.0)
gf	-69.86	kJ/mol	Joback Method
hf	-600.08	kJ/mol	Cheméo Relay (1.0)
hfus	40.18	kJ/mol	Joback Method
hvap	88.30	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-5.45		Cheméo Relay (1.0)
logp	5.027		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
tb	556.47	K	Cheméo Relay (1.0)
tc	733.75	K	Cheméo Relay (1.0)
tf	246.99	K	Cheméo Relay (1.0)
vc	0.897	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.12	J/mol×K	645.93	Joback Method
cpg	672.59	J/mol×K	674.67	Joback Method
cpg	689.29	J/mol×K	703.40	Joback Method
cpg	705.23	J/mol×K	732.14	Joback Method
cpg	720.44	J/mol×K	760.87	Joback Method
cpg	734.94	J/mol×K	789.61	Joback Method
cpg	748.76	J/mol×K	818.34	Joback Method
dvisc	0.0022449	Pa×s	337.16	Joback Method

dvisc	0.0009605	Pa×s	388.62	Joback Method
dvisc	0.0005012	Pa×s	440.08	Joback Method
dvisc	0.0002997	Pa×s	491.54	Joback Method
dvisc	0.0001976	Pa×s	543.01	Joback Method
dvisc	0.0001400	Pa×s	594.47	Joback Method
dvisc	0.0001048	Pa×s	645.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U130819&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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