

(4Z,7Z)-2-Acetoxy-4,7-tridecadiene

Inchi:	InChI=1S/C15H26O2/c1-4-5-6-7-8-9-10-11-12-13-14(2)17-15(3)16/h8-9,11-12,14H,4-7,1
InchiKey:	WBTCMXVCGSBLBM-MURFETPASA-N
Formula:	C15H26O2
SMILES:	CCCCC=CCC=CCC(C)OC(C)=O
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-0.50	kJ/mol	Joback Method
hf	-368.57	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.411		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	1605.00		NIST Webbook
rinpol	1605.00		NIST Webbook
tb	626.77	K	Joback Method
tc	808.54	K	Joback Method
tf	305.81	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.58	J/molxK	626.77	Joback Method
cpg	597.49	J/molxK	657.06	Joback Method
cpg	613.59	J/molxK	687.36	Joback Method
cpg	628.91	J/molxK	717.65	Joback Method
cpg	643.47	J/molxK	747.95	Joback Method
cpg	657.33	J/molxK	778.24	Joback Method
cpg	670.50	J/molxK	808.54	Joback Method
dvisc	0.0030582	Paxs	305.81	Joback Method

dvisc	0.0011102	Paxs	359.30	Joback Method
dvisc	0.0005240	Paxs	412.80	Joback Method
dvisc	0.0002939	Paxs	466.29	Joback Method
dvisc	0.0001856	Paxs	519.78	Joback Method
dvisc	0.0001278	Paxs	573.28	Joback Method
dvisc	0.0000937	Paxs	626.77	Joback Method

Sources

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=R413526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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