E-3-dodecenyl acetate

Inchi: InChI=1S/C14H26O2/c1-3-4-5-6-7-8-9-10-11-12-13-16-14(2)15/h10-11H,3-9,12-13H2,1-2

InchiKey: NLVAHXQJCLXFGL-ZHACJKMWSA-N

Formula: C14H26O2

SMILES: CCCCCCCCC=CCCOC(C)=O

Mol. weight [g/mol]: 226.35

Physical Properties

Property code	Value	Unit	Source
gf	-86.70	kJ/mol	Joback Method
hf	-459.87	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	55.87	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.246		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1956.00		NIST Webbook
tb	600.17	K	Joback Method
tc	774.06	K	Joback Method
tf	314.62	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.45	J/mol×K	600.17	Joback Method
cpg	622.98	J/mol×K	745.08	Joback Method
cpg	609.24	J/mol×K	716.10	Joback Method
cpg	594.83	J/mol×K	687.12	Joback Method
cpg	579.75	J/mol×K	658.13	Joback Method

cpg	563.96	J/mol×K	629.15	Joback Method
cpg	636.08	J/mol×K	774.06	Joback Method
dvisc	0.0001309	Pa×s	600.17	Joback Method
dvisc	0.0001737	Pa×s	552.58	Joback Method
dvisc	0.0002432	Pa×s	504.99	Joback Method
dvisc	0.0003653	Pa×s	457.40	Joback Method
dvisc	0.0006028	Pa×s	409.80	Joback Method
dvisc	0.0011349	Pa×s	362.21	Joback Method
dvisc	0.0025872	Pa×s	314.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R86663&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from: