Z-4-dodecenyl acetate

Inchi: InChI=1S/C14H26O2/c1-3-4-5-6-7-8-9-10-11-12-13-16-14(2)15/h9-10H,3-8,11-13H2,1-2
InchiKey: HVFBMRUBJRAFIN-KTKRTIGZSA-N
Formula: C14H26O2
SMILES: CCCCCCCC=CCCCOC(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	1589.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1520.00		NIST Webbook
ripol	1963.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1963.00		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	563.96	J/mol×K	629.15	Joback Method
cpg	579.75	J/mol×K	658.13	Joback Method

cpg	594.83	J/mol×K	687.12	Joback Method
cpg	609.24	J/mol×K	716.10	Joback Method
cpg	622.98	J/mol×K	745.08	Joback Method
cpg	636.08	J/mol×K	774.06	Joback Method
dvisc	0.0025872	Pa×s	314.62	Joback Method
dvisc	0.0011349	Pa×s	362.21	Joback Method
dvisc	0.0006028	Pa×s	409.80	Joback Method
dvisc	0.0003653	Pa×s	457.40	Joback Method
dvisc	0.0002432	Pa×s	504.99	Joback Method
dvisc	0.0001737	Pa×s	552.58	Joback Method
dvisc	0.0001309	Pa×s	600.17	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=R86944&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
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