Undecanoic acid, 1-methylethyl ester

Other names: isopropyl undecanoate
Inchi: InChI=1S/C14H28O2/c1-4-5-6-7-8-9-10-11-12-14(15)16-13(2)3/h13H,4-12H2,1-3H3
InchiKey: KJRRQERTCPYNMS-UHFFFAOYSA-N
Formula: C14H28O2
SMILES: CCCCCCCCCCC(=O)OC(C)C
Mol. weight [g/mol]: 228.37
CAS: 50638-98-7

Physical Properties

Property code	Value	Unit	Source
gf	-169.36	kJ/mol	Joback Method
hf	-582.37	kJ/mol	Joback Method
hfus	31.28	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.469		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1516.00		NIST Webbook
rinpol	1516.00		NIST Webbook
ripol	1715.00		NIST Webbook
ripol	1715.00		NIST Webbook
tb	595.57	K	Joback Method
tc	766.26	K	Joback Method
tf	304.70	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.35	J/mol×K	595.57	Joback Method
cpg	646.34	J/mol×K	737.81	Joback Method
cpg	631.92	J/mol×K	709.36	Joback Method
cpg	616.82	J/mol×K	680.91	Joback Method

cpg	601.04	J/mol×K	652.47	Joback Method
cpg	584.55	J/mol×K	624.02	Joback Method
cpg	660.10	J/mol×K	766.26	Joback Method
dvisc	0.0001432	Pa×s	595.57	Joback Method
dvisc	0.0001938	Pa×s	547.09	Joback Method
dvisc	0.0002782	Pa×s	498.61	Joback Method
dvisc	0.0004318	Pa×s	450.13	Joback Method
dvisc	0.0007451	Pa×s	401.66	Joback Method
dvisc	0.0014934	Pa×s	353.18	Joback Method
dvisc	0.0037349	Pa×s	304.70	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=C50638987&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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