

Undecanoic acid, isobutyl ester

Other names:	Isobutyl undecanoate
Inchi:	InChI=1S/C15H30O2/c1-4-5-6-7-8-9-10-11-12-15(16)17-13-14(2)3/h14H,4-13H2,1-3H3
InchiKey:	CTPIEDAGOVPLZ-UHFFFAOYSA-N
Formula:	C15H30O2
SMILES:	CCCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	242.40

Physical Properties

Property code	Value	Unit	Source
gf	-160.94	kJ/mol	Joback Method
hf	-603.01	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.716		Crippen Method
mvol	229.650	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1627.00		NIST Webbook
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tb	618.45	K	Joback Method
tc	788.43	K	Joback Method
tf	315.97	K	Joback Method
vc	0.893	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.09	J/mol×K	618.45	Joback Method
cpg	638.80	J/mol×K	646.78	Joback Method
cpg	655.75	J/mol×K	675.11	Joback Method
cpg	671.98	J/mol×K	703.44	Joback Method
cpg	687.48	J/mol×K	731.77	Joback Method
cpg	702.28	J/mol×K	760.10	Joback Method
cpg	716.38	J/mol×K	788.43	Joback Method

dvisc	0.0034492	Paxs	315.97	Joback Method
dvisc	0.0013649	Paxs	366.38	Joback Method
dvisc	0.0006759	Paxs	416.80	Joback Method
dvisc	0.0003895	Paxs	467.21	Joback Method
dvisc	0.0002499	Paxs	517.62	Joback Method
dvisc	0.0001735	Paxs	568.04	Joback Method
dvisc	0.0001278	Paxs	618.45	Joback Method

Sources

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=U405158&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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