

Tridecanoic acid, isobutyl ester

Other names:	Isobutyl tridecanoate
Inchi:	InChI=1S/C17H34O2/c1-4-5-6-7-8-9-10-11-12-13-14-17(18)19-15-16(2)3/h16H,4-15H2,1
InchiKey:	DBSNEMMWHLXCPX-UHFFFAOYSA-N
Formula:	C17H34O2
SMILES:	CCCCCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	270.45

Physical Properties

Property code	Value	Unit	Source
gf	-144.10	kJ/mol	Joback Method
hf	-644.29	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.497		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	1826.00		NIST Webbook
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tb	664.21	K	Joback Method
tc	833.82	K	Joback Method
tf	338.51	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.67	J/molxK	664.21	Joback Method
cpg	751.27	J/molxK	692.48	Joback Method
cpg	769.05	J/molxK	720.75	Joback Method
cpg	786.03	J/molxK	749.02	Joback Method
cpg	802.22	J/molxK	777.28	Joback Method
cpg	817.65	J/molxK	805.55	Joback Method
cpg	832.34	J/molxK	833.82	Joback Method

dvisc	0.0028787	Paxs	338.51	Joback Method
dvisc	0.0011177	Paxs	392.79	Joback Method
dvisc	0.0005461	Paxs	447.08	Joback Method
dvisc	0.0003116	Paxs	501.36	Joback Method
dvisc	0.0001983	Paxs	555.64	Joback Method
dvisc	0.0001368	Paxs	609.93	Joback Method
dvisc	0.0001003	Paxs	664.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405160&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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