Pentadecanoic acid, 3-methylbutyl ester

Other names:	iso-Amyl n-decanoate
	3-Methylbuthyl ester of pentadecanoic acid
	3-Methylbutyl decanoate
	Isoamyl decanoate
	Isopentyl decanoate
	3-Methylbuthyl ester pentadecanoic acid
Inchi:	InChI=1S/C15H30O2/c1-4-5-6-7-8-9-10-11-15(16)17-13-12-14(2)3/h14H,4-13H2,1-3H3
InchiKey:	XDOGFYDZGUDBQY-UHFFFAOYSA-N
Formula:	C15H30O2
SMILES:	CCCCCCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	242.40
CAS:	2306-91-4

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
mcvol	229.650	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1646.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1653.40		NIST Webbook
rinpol	1615.00		NIST Webbook

rinpol	1627.00		NIST Webbook
ripol	1864.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1848.00		NIST Webbook
ripol	1853.00		NIST Webbook
ripol	1859.00		NIST Webbook
ripol	1851.00		NIST Webbook
ripol	1859.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1864.00		NIST Webbook
ripol	1866.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1856.00		NIST Webbook
ripol	1861.00		NIST Webbook
tb	618.45	K	Joback Method
tc	788.43	K	Joback Method
tf	315.97	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.09	J/mol×K	618.45	Joback Method
cpg	702.28	J/mol×K	760.10	Joback Method
cpg	687.48	J/mol×K	731.77	Joback Method
cpg	671.98	J/mol×K	703.44	Joback Method
cpg	655.75	J/mol×K	675.11	Joback Method
cpg	638.80	J/mol×K	646.78	Joback Method
cpg	716.38	J/mol×K	788.43	Joback Method
dvisc	0.0001278	Pa×s	618.45	Joback Method
dvisc	0.0001735	Pa×s	568.04	Joback Method
dvisc	0.0002499	Pa×s	517.62	Joback Method
dvisc	0.0003895	Pa×s	467.21	Joback Method
dvisc	0.0006759	Pa×s	416.80	Joback Method
dvisc	0.0013649	Pa×s	366.38	Joback Method
dvisc	0.0034492	Pa×s	315.97	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=C2306914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume