ISOBUTYL DECANOATE

Other names:	Decanoic acid, 2-methylpropyl ester
	Decanoic acid, isobutyl ester
	Isobutyl decanoate
	2-Methylpropyl decanoate
	Isobutyl caprate
Inchi:	InChI=1S/C14H28O2/c1-4-5-6-7-8-9-10-11-14(15)16-12-13(2)3/h13H,4-12H2,1-3H3
InchiKey:	AXTPGRJJIGEOOY-UHFFFAOYSA-N
Formula:	C14H28O2
SMILES:	CCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	228.38

Physical Properties

Property code	Value	Unit	Source
af	0.7355		Cheméo Relay (1.0)
hf	-661.97	kJ/mol	Cheméo Relay (1.0)
hfus	31.28	kJ/mol	Joback Method
hvap	67.90	kJ/mol	Cheméo Relay (1.0)
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-4.74		Cheméo Relay (1.0)
logp	4.326		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1545.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1549.50		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1549.50		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1545.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1751.00		NIST Webbook

ripol	1750.00		NIST Webbook
ripol	1756.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1750.00		NIST Webbook
tb	530.56	K	Cheméo Relay (1.0)
tc	700.10	K	Cheméo Relay (1.0)
tf	244.24	K	Cheméo Relay (1.0)
vc	0.833	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.35	J/mol×K	595.57	Joback Method
cpg	660.10	J/mol×K	766.26	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
dvisc	0.0004318	Pa×s	450.13	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	0.0037349	Pa×s	304.70	Joback Method
dvisc	0.0007451	Pa×s	401.66	Joback Method
dvisc	0.0014934	Pa×s	353.18	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30673382&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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