Propanoic acid, 2-methyl-, decyl ester

Other names:	Decyl isobutanoate
	Decyl isobutyrate
	Isobutyric acid, decyl ester
Inchi:	InChI=1S/C14H28O2/c1-4-5-6-7-8-9-10-11-12-16-14(15)13(2)3/h13H,4-12H2,1-3H3
InchiKey:	HGOZECVJNYXKMC-UHFFFAOYSA-N
Formula:	C14H28O2
SMILES:	CCCCCCCCCCOC(=O)C(C)C
Mol. weight [g/mol]:	228.37
CAS:	5454-22-8

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	-4.30		Crippen Method
logp	4.326		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1590.00		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	584.55	J/mol×K	624.02	Joback Method
cpg	601.04	J/mol×K	652.47	Joback Method
cpg	616.82	J/mol×K	680.91	Joback Method
cpg	631.92	J/mol×K	709.36	Joback Method

cpg	646.34	J/mol×K	737.81	Joback Method
cpg	660.10	J/mol×K	766.26	Joback Method
dvisc	0.0037349	Pa×s	304.70	Joback Method
dvisc	0.0014934	Pa×s	353.18	Joback Method
dvisc	0.0007451	Pa×s	401.66	Joback Method
dvisc	0.0004318	Pa×s	450.13	Joback Method
dvisc	0.0002782	Pa×s	498.61	Joback Method
dvisc	0.0001938	Pa×s	547.09	Joback Method
dvisc	0.0001432	Pa×s	595.57	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48256e+01
Coeff. B	-4.61965e+03
Coeff. C	-9.07560e+01
Temperature range (K), min.	408.52
Temperature range (K), max.	576.31

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5454228&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

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

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
pvap:	Vapor 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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