Propanoic acid, 2-methyl-, octyl ester

Other names:	Caprylyl isobutyrate
	ENT 24265
	Isobutyric acid, octyl ester
	Octyl Isobutyrate
	Octyl isobutanoate
	n-Octyl isobutyrate
	octyl 2-methyl propanoate
Inchi:	InChI=1S/C12H24O2/c1-4-5-6-7-8-9-10-14-12(13)11(2)3/h11H,4-10H2,1-3H3
InchiKey:	PQCYCHFQWMNQRJ-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCCCOC(=O)C(C)C
Mol. weight [g/mol]:	200.32
CAS:	109-15-9

Physical Properties

Property code	Value	Unit	Source
gf	-186.20	kJ/mol	Joback Method
hf	-541.09	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	51.07	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.546		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1348.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1329.00		NIST Webbook

rinpol	1343.90		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1332.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1535.00		NIST Webbook
tb	549.81	K	Joback Method
tc	722.69	K	Joback Method
tf	282.16	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.44	J/mol×K	549.81	Joback Method
cpg	538.20	J/mol×K	693.88	Joback Method
cpg	524.69	J/mol×K	665.07	Joback Method
cpg	510.57	J/mol×K	636.25	Joback Method
cpg	495.83	J/mol×K	607.44	Joback Method
cpg	480.46	J/mol×K	578.62	Joback Method
cpg	551.11	J/mol×K	722.69	Joback Method
dvisc	0.0001764	Pa×s	549.81	Joback Method
dvisc	0.0002373	Pa×s	505.20	Joback Method
dvisc	0.0003381	Pa×s	460.59	Joback Method
dvisc	0.0005197	Pa×s	415.99	Joback Method
dvisc	0.0008857	Pa×s	371.38	Joback Method
dvisc	0.0017460	Pa×s	326.77	Joback Method
dvisc	0.0042661	Pa×s	282.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48628e+01

Coeff. B	-4.39564e+03
Coeff. C	-8.21380e+01
Temperature range (K), min.	383.72
Temperature range (K), max.	542.35

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109159&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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