Octanoic acid, octyl ester

Other names: Octyl caprylate
Octyl octanoate
n-Octyl caprylate
Inchi: InChI=1S/C16H32O2/c1-3-5-7-9-11-13-15-18-16(17)14-12-10-8-6-4-2/h3-15H2,1-2H3
InchiKey: DJNTZVRUYMHBTD-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CCCCCCCCOC(=O)CCCCCCC
Mol. weight [g/mol]: 256.42
CAS: 2306-88-9

Physical Properties

Property code	Value	Unit	Source
gf	-150.08	kJ/mol	Joback Method
hf	-618.37	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.251		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1763.00		NIST Webbook
rinpol	1767.00		NIST Webbook
rinpol	1779.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1767.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1779.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	1998.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	1998.00		NIST Webbook
tb	571.00 ± 6.00	K	NIST Webbook
tb	479.10 ± 3.00	K	NIST Webbook
tb	580.00 ± 1.00	K	NIST Webbook
tc	809.14	K	Joback Method
tf	255.07 ± 0.20	K	NIST Webbook
tf	258.10 ± 1.00	K	NIST Webbook

tf	263.00 ± 4.00	K	NIST Webbook
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.85	J/mol×K	641.77	Joback Method
cpg	693.74	J/mol×K	669.66	Joback Method
cpg	710.87	J/mol×K	697.56	Joback Method
cpg	727.27	J/mol×K	725.45	Joback Method
cpg	742.94	J/mol×K	753.35	Joback Method
cpg	757.90	J/mol×K	781.24	Joback Method
cpg	772.16	J/mol×K	809.14	Joback Method
dvisc	0.0024033	Pa×s	342.24	Joback Method
dvisc	0.0010661	Pa×s	392.16	Joback Method
dvisc	0.0005682	Pa×s	442.08	Joback Method
dvisc	0.0003441	Pa×s	492.00	Joback Method
dvisc	0.0002286	Pa×s	541.93	Joback Method
dvisc	0.0001627	Pa×s	591.85	Joback Method
dvisc	0.0001221	Pa×s	641.77	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51643e+01
Coeff. B	-5.03702e+03
Coeff. C	-1.02376e+02
Temperature range (K), min.	440.96
Temperature range (K), max.	613.60

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2306889&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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