Hexanoic acid, octyl ester

Other names: Octyl caproate
Octyl hexanoate
n-Octyl hexanoate
Inchi: InChI=1S/C14H28O2/c1-3-5-7-8-9-11-13-16-14(15)12-10-6-4-2/h3-13H2,1-2H3
InchiKey: CMNMHJVRZHGAAK-UHFFFAOYSA-N
Formula: C14H28O2
SMILES: CCCCCCCCOC(=O)CCCCC
Mol. weight [g/mol]: 228.37
CAS: 4887-30-3

Physical Properties

Property code	Value	Unit	Source
gf	-166.92	kJ/mol	Joback Method
hf	-577.09	kJ/mol	Joback Method
hfus	34.80	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.470		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	1567.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
ripol	1829.00		NIST Webbook
ripol	1815.00		NIST Webbook
ripol	1829.00		NIST Webbook
ripol	1829.00		NIST Webbook
tb	548.40 ± 2.00	K	NIST Webbook
tb	543.00 ± 4.00	K	NIST Webbook
tb	548.40 ± 1.50	K	NIST Webbook
tc	764.02	K	Joback Method
tf	245.10 ± 1.00	K	NIST Webbook

vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.02	J/mol×K	596.01	Joback Method
cpg	583.90	J/mol×K	624.01	Joback Method
cpg	600.10	J/mol×K	652.01	Joback Method
cpg	615.63	J/mol×K	680.02	Joback Method
cpg	630.49	J/mol×K	708.02	Joback Method
cpg	644.71	J/mol×K	736.02	Joback Method
cpg	658.29	J/mol×K	764.02	Joback Method
dvisc	0.0027735	Pa×s	319.70	Joback Method
dvisc	0.0012632	Pa×s	365.75	Joback Method
dvisc	0.0006860	Pa×s	411.80	Joback Method
dvisc	0.0004212	Pa×s	457.86	Joback Method
dvisc	0.0002827	Pa×s	503.91	Joback Method
dvisc	0.0002029	Pa×s	549.96	Joback Method
dvisc	0.0001532	Pa×s	596.01	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51122e+01
Coeff. B	-4.77330e+03
Coeff. C	-9.35360e+01
Temperature range (K), min.	415.52
Temperature range (K), max.	580.57

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4887303&Units=SI

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