Pentanoic acid, octyl ester

Other names: Octyl pentanoate
Valeric acid, octyl ester
octyl valerate
Inchi: InChI=1S/C13H26O2/c1-3-5-7-8-9-10-12-15-13(14)11-6-4-2/h3-12H2,1-2H3
InchiKey: OUYCCOBIJYUMAK-UHFFFAOYSA-N
Formula: C13H26O2
SMILES: CCCCCCCCOC(=O)CCCC
Mol. weight [g/mol]: 214.34
CAS: 5451-85-4

Physical Properties

Property code	Value	Unit	Source
gf	-175.34	kJ/mol	Joback Method
hf	-556.45	kJ/mol	Joback Method
hfus	32.21	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.080		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	1474.00		NIST Webbook
rinpol	1474.00		NIST Webbook
ripol	1719.00		NIST Webbook
ripol	1719.00		NIST Webbook
tb	533.40 ± 2.00	K	NIST Webbook
tb	534.75 ± 0.30	K	NIST Webbook
tc	741.92	K	Joback Method
tf	230.90 ± 0.50	K	NIST Webbook
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.80	J/mol×K	573.13	Joback Method

cpg	531.11	J/mol×K	601.26	Joback Method
cpg	546.77	J/mol×K	629.39	Joback Method
cpg	561.79	J/mol×K	657.52	Joback Method
cpg	576.19	J/mol×K	685.66	Joback Method
cpg	589.97	J/mol×K	713.79	Joback Method
cpg	603.14	J/mol×K	741.92	Joback Method
dvisc	0.0029408	Pa×s	308.43	Joback Method
dvisc	0.0013589	Pa×s	352.55	Joback Method
dvisc	0.0007456	Pa×s	396.66	Joback Method
dvisc	0.0004613	Pa×s	440.78	Joback Method
dvisc	0.0003115	Pa×s	484.90	Joback Method
dvisc	0.0002245	Pa×s	529.01	Joback Method
dvisc	0.0001702	Pa×s	573.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51157e+01
Coeff. B	-4.67070e+03
Coeff. C	-8.98100e+01
Temperature range (K), min.	404.80
Temperature range (K), max.	566.21

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1131.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5451854&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