

Heptanoic acid, octyl ester

Other names:	octyl heptanoate
Inchi:	InChI=1S/C15H30O2/c1-3-5-7-9-10-12-14-17-15(16)13-11-8-6-4-2/h3-14H2,1-2H3
InchiKey:	XAZROQGRFWCMBU-UHFFFAOYSA-N
Formula:	C15H30O2
SMILES:	CCCCCCCCOC(=O)CCCCCC
Mol. weight [g/mol]:	242.40
CAS:	5132-75-2

Physical Properties

Property code	Value	Unit	Source
gf	-158.50	kJ/mol	Joback Method
hf	-597.73	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.861		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
tb	563.60 ± 5.00	K	NIST Webbook
tb	563.90 ± 1.00	K	NIST Webbook
tc	786.41	K	Joback Method
tf	251.70 ± 1.00	K	NIST Webbook
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.74	J/molxK	618.89	Joback Method
cpg	700.70	J/molxK	758.49	Joback Method
cpg	686.10	J/molxK	730.57	Joback Method
cpg	670.81	J/molxK	702.65	Joback Method
cpg	654.83	J/molxK	674.73	Joback Method
cpg	638.14	J/molxK	646.81	Joback Method
cpg	714.65	J/molxK	786.41	Joback Method

dvisc	0.0001371	Paxs	618.89	Joback Method
dvisc	0.0001822	Paxs	570.90	Joback Method
dvisc	0.0002549	Paxs	522.92	Joback Method
dvisc	0.0003819	Paxs	474.93	Joback Method
dvisc	0.0006264	Paxs	426.94	Joback Method
dvisc	0.0011647	Paxs	378.96	Joback Method
dvisc	0.0025922	Paxs	330.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50916e+01
Coeff. B	-4.88256e+03
Coeff. C	-9.77060e+01
Temperature range (K), min.	427.52
Temperature range (K), max.	596.94

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/ci9903071
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=C5132752&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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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