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
af	0.8001		Cheméo Relay (1.0)
hf	-670.18	kJ/mol	Cheméo Relay (1.0)
hfus	37.39	kJ/mol	Joback Method
hvap	74.98	kJ/mol	Cheméo Relay (1.0)
ie	9.51	eV	Cheméo Relay (1.0)
log10ws	-5.07		Cheméo Relay (1.0)
logp	4.861		Crippen Method
mcvol	229.650	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
tb	563.90 ± 1.00	K	NIST Webbook
tb	563.60 ± 5.00	K	NIST Webbook
tc	728.62	K	Cheméo Relay (1.0)
tf	251.70 ± 1.00	K	NIST Webbook
vc	0.897	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	714.65	J/mol×K	786.41	Joback Method
dvisc	0.0025922	Pa×s	330.97	Joback Method
dvisc	0.0011647	Pa×s	378.96	Joback Method
dvisc	0.0006264	Pa×s	426.94	Joback Method
dvisc	0.0003819	Pa×s	474.93	Joback Method
dvisc	0.0002549	Pa×s	522.92	Joback Method
dvisc	0.0001822	Pa×s	570.90	Joback Method
dvisc	0.0001371	Pa×s	618.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5132752&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume