Heptyl caprylate

Other names:	Heptyl octanoate
	Octanoic acid, heptyl ester
	n-Heptyl n-octanoate
Inchi:	InChI=1S/C15H30O2/c1-3-5-7-9-11-13-15(16)17-14-12-10-8-6-4-2/h3-14H2,1-2H3
InchiKey:	TZXWLJYLYILFGM-UHFFFAOYSA-N
Formula:	C15H30O2
SMILES:	CCCCCCCOC(=O)CCCCCCC
Mol. weight [g/mol]:	242.40
CAS:	4265-97-8

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
rinpol	1666.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1666.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1892.00		NIST Webbook
tb	563.80 ± 1.00	K	NIST Webbook
tb	572.00 ± 4.00	K	NIST Webbook
tc	786.41	K	Joback Method
tf	267.00 ± 2.00	K	NIST Webbook
tf	263.00 ± 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/mol×K	618.89	Joback Method
cpg	700.70	J/mol×K	758.49	Joback Method
cpg	686.10	J/mol×K	730.57	Joback Method
cpg	670.81	J/mol×K	702.65	Joback Method
cpg	654.83	J/mol×K	674.73	Joback Method
cpg	638.14	J/mol×K	646.81	Joback Method
cpg	714.65	J/mol×K	786.41	Joback Method
dvisc	0.0001371	Pa×s	618.89	Joback Method
dvisc	0.0001822	Pa×s	570.90	Joback Method
dvisc	0.0002549	Pa×s	522.92	Joback Method
dvisc	0.0003819	Pa×s	474.93	Joback Method
dvisc	0.0006264	Pa×s	426.94	Joback Method
dvisc	0.0011647	Pa×s	378.96	Joback Method
dvisc	0.0025922	Pa×s	330.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51384e+01
Coeff. B	-4.90189e+03
Coeff. C	-9.78450e+01
Temperature range (K), min.	427.92
Temperature range (K), max.	596.67

Sources

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=C4265978&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

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

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