

Nonanoic acid, heptyl ester

Other names:	heptyl nonan-1-oate heptyl nonanoate
Inchi:	InChI=1S/C16H32O2/c1-3-5-7-9-10-12-14-16(17)18-15-13-11-8-6-4-2/h3-15H2,1-2H3
InchiKey:	ARSLOAKOWGOSEX-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]:	256.42
CAS:	71605-85-1

Physical Properties

Property code	Value	Unit	Source
gf	-150.08	kJ/mol	Joback Method
hf	-618.37	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.251		Crippen Method
mvol	243.740	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
tb	641.77	K	Joback Method
tc	809.14	K	Joback Method
tf	257.61 ± 0.20	K	NIST Webbook
vc	0.956	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.85	J/mol×K	641.77	Joback Method
cpg	693.74	J/mol×K	669.66	Joback Method
cpg	710.87	J/mol×K	697.56	Joback Method
cpg	727.27	J/mol×K	725.45	Joback Method
cpg	742.94	J/mol×K	753.35	Joback Method

cpg	757.90	J/molxK	781.24	Joback Method
cpg	772.16	J/molxK	809.14	Joback Method
dvisc	0.0024033	Paxs	342.24	Joback Method
dvisc	0.0010661	Paxs	392.16	Joback Method
dvisc	0.0005682	Paxs	442.08	Joback Method
dvisc	0.0003441	Paxs	492.00	Joback Method
dvisc	0.0002286	Paxs	541.93	Joback Method
dvisc	0.0001627	Paxs	591.85	Joback Method
dvisc	0.0001221	Paxs	641.77	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49106e+01
Coeff. B	-4.87568e+03
Coeff. C	-9.90960e+01
Temperature range (K), min.	432.52
Temperature range (K), max.	607.02

Sources

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=C71605851&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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