

Nonanoic acid, hexyl ester

Other names:	hexyl nonan-1-oate
Inchi:	InChI=1S/C15H30O2/c1-3-5-7-9-10-11-13-15(16)17-14-12-8-6-4-2/h3-14H2,1-2H3
InchiKey:	GPHBCFMWKGZPRP-UHFFFAOYSA-N
Formula:	C15H30O2
SMILES:	CCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]:	242.40
CAS:	6561-39-3

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	1668.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1684.80		NIST Webbook
rinpol	1684.80		NIST Webbook
ripol	1900.00		NIST Webbook
tb	618.89	K	Joback Method
tc	786.41	K	Joback Method
tf	330.97	K	Joback Method
vc	0.899	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	620.74	J/molxK	618.89	Joback Method
cpg	638.14	J/molxK	646.81	Joback Method
cpg	654.83	J/molxK	674.73	Joback Method
cpg	670.81	J/molxK	702.65	Joback Method
cpg	686.10	J/molxK	730.57	Joback Method
cpg	700.70	J/molxK	758.49	Joback Method
cpg	714.65	J/molxK	786.41	Joback Method
dvisc	0.0025922	Paxs	330.97	Joback Method
dvisc	0.0011647	Paxs	378.96	Joback Method
dvisc	0.0006264	Paxs	426.94	Joback Method
dvisc	0.0003819	Paxs	474.93	Joback Method
dvisc	0.0002549	Paxs	522.92	Joback Method
dvisc	0.0001822	Paxs	570.90	Joback Method
dvisc	0.0001371	Paxs	618.89	Joback Method

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=C6561393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical 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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