

(E)-2-Hexenyl nonanoate

Inchi:	InChI=1S/C15H28O2/c1-3-5-7-9-10-11-13-15(16)17-14-12-8-6-4-2/h8,12H,3-7,9-11,13-15H
InchiKey:	LSKQJQBOOYBILS-XYOKQWHBSA-N
Formula:	C15H28O2
SMILES:	CCCC=CCOC(=O)CCCCCCCC
Mol. weight [g/mol]:	240.38

Physical Properties

Property code	Value	Unit	Source
gf	-78.28	kJ/mol	Joback Method
hf	-480.51	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	58.10	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.636		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
ripol	1673.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1953.00		NIST Webbook
tb	623.05	K	Joback Method
tc	796.03	K	Joback Method
tf	325.89	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.59	J/molxK	623.05	Joback Method
cpg	617.60	J/molxK	651.88	Joback Method
cpg	633.86	J/molxK	680.71	Joback Method
cpg	649.40	J/molxK	709.54	Joback Method
cpg	664.23	J/molxK	738.37	Joback Method
cpg	678.37	J/molxK	767.20	Joback Method

cpg	691.85	J/molxK	796.03	Joback Method
dvisc	0.0024199	Paxs	325.89	Joback Method
dvisc	0.0010480	Paxs	375.42	Joback Method
dvisc	0.0005516	Paxs	424.94	Joback Method
dvisc	0.0003319	Paxs	474.47	Joback Method
dvisc	0.0002199	Paxs	524.00	Joback Method
dvisc	0.0001564	Paxs	573.52	Joback Method
dvisc	0.0001174	Paxs	623.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R409715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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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