

n-Heptyl hexanoate

Other names:	Hexanoic acid, heptyl ester heptyl hexanoate
Inchi:	InChI=1S/C13H26O2/c1-3-5-7-8-10-12-15-13(14)11-9-6-4-2/h3-12H2,1-2H3
InchiKey:	QEKCBKVWQYEUGY-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CCCCCCCOC(=O)CCCCC
Mol. weight [g/mol]:	214.34
CAS:	6976-72-3

Physical Properties

Property code	Value	Unit	Source
gf	-175.34	kJ/mol	Joback Method
hf	-556.45	kJ/mol	Joback Method
hfus	32.21	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.080		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	1482.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1448.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1683.00		NIST Webbook
tb	532.60 ± 3.00	K	NIST Webbook
tb	534.12 ± 0.30	K	NIST Webbook
tc	741.92	K	Joback Method
tf	238.90 ± 0.50	K	NIST Webbook
vc	0.787	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.80	J/molxK	573.13	Joback Method
cpg	531.11	J/molxK	601.26	Joback Method
cpg	546.77	J/molxK	629.39	Joback Method
cpg	561.79	J/molxK	657.52	Joback Method
cpg	576.19	J/molxK	685.66	Joback Method
cpg	589.97	J/molxK	713.79	Joback Method
cpg	603.14	J/molxK	741.92	Joback Method
dvisc	0.0029408	Paxs	308.43	Joback Method
dvisc	0.0013589	Paxs	352.55	Joback Method
dvisc	0.0007456	Paxs	396.66	Joback Method
dvisc	0.0004613	Paxs	440.78	Joback Method
dvisc	0.0003115	Paxs	484.90	Joback Method
dvisc	0.0002245	Paxs	529.01	Joback Method
dvisc	0.0001702	Paxs	573.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51174e+01
Coeff. B	-4.66659e+03
Coeff. C	-8.96440e+01
Temperature range (K), min.	404.32
Temperature range (K), max.	565.54

Sources

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=C6976723&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/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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ripol:	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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