

Heptanoic acid, heptyl ester

Other names:	Heptyl heptanoate Heptyl heptoate
Inchi:	InChI=1S/C14H28O2/c1-3-5-7-9-11-13-16-14(15)12-10-8-6-4-2/h3-13H2,1-2H3
InchiKey:	QOIBPAJVVFEPE-UHFFFAOYSA-N
Formula:	C14H28O2
SMILES:	CCCCCCCCOC(=O)CCCCC
Mol. weight [g/mol]:	228.37
CAS:	624-09-9

Physical Properties

Property code	Value	Unit	Source
gf	-166.92	kJ/mol	Joback Method
hf	-577.09	kJ/mol	Joback Method
hfus	34.80	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.470		Crippen Method
mvol	215.560	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
tb	550.00 ± 3.00	K	NIST Webbook
tb	544.00 ± 4.00	K	NIST Webbook
tb	547.80 ± 3.00	K	NIST Webbook
tb	550.36 ± 0.30	K	NIST Webbook
tc	764.02	K	Joback Method
tf	239.90 ± 0.50	K	NIST Webbook
vc	0.844	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.02	J/mol×K	596.01	Joback Method
cpg	583.90	J/mol×K	624.01	Joback Method
cpg	600.10	J/mol×K	652.01	Joback Method
cpg	615.63	J/mol×K	680.02	Joback Method

cpg	630.49	J/molxK	708.02	Joback Method
cpg	644.71	J/molxK	736.02	Joback Method
cpg	658.29	J/molxK	764.02	Joback Method
dvisc	0.0027735	Paxs	319.70	Joback Method
dvisc	0.0012632	Paxs	365.75	Joback Method
dvisc	0.0006860	Paxs	411.80	Joback Method
dvisc	0.0004212	Paxs	457.86	Joback Method
dvisc	0.0002827	Paxs	503.91	Joback Method
dvisc	0.0002029	Paxs	549.96	Joback Method
dvisc	0.0001532	Paxs	596.01	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51178e+01
Coeff. B	-4.79058e+03
Coeff. C	-9.40920e+01
Temperature range (K), min.	417.12
Temperature range (K), max.	582.61

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<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>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C624099&Units=SI>

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

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