Heptanoic acid, pentyl ester

Other names: pentyl heptanoate
Inchi: InChI=1S/C12H24O2/c1-3-5-7-8-10-12(13)14-11-9-6-4-2/h3-11H2,1-2H3
InchiKey: PSQMUBJRXIGVIT-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CCCCCCC(=O)OCCCCC
Mol. weight [g/mol]: 200.32
CAS: 7493-82-5

Physical Properties

Property code	Value	Unit	Source
gf	-183.76	kJ/mol	Joback Method
hf	-535.81	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	51.46	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.690		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1375.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1600.00		NIST Webbook
tb	518.59 ± 0.30	K	NIST Webbook
tb	396.15 ± 5.00	K	NIST Webbook
tc	720.05	K	Joback Method
tf	223.70 ± 0.50	K	NIST Webbook
tf	224.20 ± 0.80	K	NIST Webbook
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.17	J/mol×K	550.25	Joback Method
cpg	536.51	J/mol×K	691.75	Joback Method
cpg	523.23	J/mol×K	663.45	Joback Method

cpg	509.36	J/mol×K	635.15	Joback Method
cpg	494.90	J/mol×K	606.85	Joback Method
cpg	479.84	J/mol×K	578.55	Joback Method
cpg	549.22	J/mol×K	720.05	Joback Method
dvisc	0.0001878	Pa×s	550.25	Joback Method
dvisc	0.0002467	Pa×s	508.07	Joback Method
dvisc	0.0003406	Pa×s	465.89	Joback Method
dvisc	0.0005012	Pa×s	423.70	Joback Method
dvisc	0.0008035	Pa×s	381.52	Joback Method
dvisc	0.0014485	Pa×s	339.34	Joback Method
dvisc	0.0030867	Pa×s	297.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50918e+01
Coeff. B	-4.53798e+03
Coeff. C	-8.53070e+01
Temperature range (K), min.	391.84
Temperature range (K), max.	549.30

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=C7493825&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/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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