

2-Heptenoic acid, pentyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H22O2/c1-3-5-7-8-10-12(13)14-11-9-6-4-2/h8,10H,3-7,9,11H2,1-2H3/b10-4

FKZKVHGWHGOBGP-CSKARUKUSA-N

C12H22O2

CCCCC=CC(=O)OCCCCC

198.30

Physical Properties

Property code	Value	Unit	Source
gf	-103.54	kJ/mol	Joback Method
hf	-418.59	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1454.00		NIST Webbook
tb	554.41	K	Joback Method
tc	730.90	K	Joback Method
tf	292.08	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.74	J/mol×K	554.41	Joback Method
cpg	461.06	J/mol×K	583.82	Joback Method
cpg	475.72	J/mol×K	613.24	Joback Method
cpg	489.74	J/mol×K	642.65	Joback Method
cpg	503.13	J/mol×K	672.07	Joback Method
cpg	515.92	J/mol×K	701.48	Joback Method
cpg	528.11	J/mol×K	730.90	Joback Method
dvisc	0.0028734	Pa×s	292.08	Joback Method
dvisc	0.0012967	Pa×s	335.80	Joback Method

dvisc	0.0007029	Pa×s	379.52	Joback Method
dvisc	0.0004324	Pa×s	423.25	Joback Method
dvisc	0.0002914	Pa×s	466.97	Joback Method
dvisc	0.0002101	Pa×s	510.69	Joback Method
dvisc	0.0001595	Pa×s	554.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406090&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

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

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