Heptyl isopentanoate

Other names: heptyl 3-methylbutanoate
heptyl isovalerate
Inchi: InChI=1S/C12H24O2/c1-4-5-6-7-8-9-14-12(13)10-11(2)3/h11H,4-10H2,1-3H3
InchiKey: NPBMPHKEFVCCEY-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CCCCCCCOC(=O)CC(C)C
Mol. weight [g/mol]: 200.32
CAS: 56423-43-9

Physical Properties

Property code	Value	Unit	Source
gf	-186.20	kJ/mol	Joback Method
hf	-541.09	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	51.07	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.546		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	1340.60		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1340.60		NIST Webbook
rinpol	1338.00		NIST Webbook
rinpol	1338.00		NIST Webbook
tb	549.81	K	Joback Method
tc	722.69	K	Joback Method
tf	282.16	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.44	J/mol×K	549.81	Joback Method
cpg	538.20	J/mol×K	693.88	Joback Method

cpg	524.69	J/mol×K	665.07	Joback Method
cpg	510.57	J/mol×K	636.25	Joback Method
cpg	495.83	J/mol×K	607.44	Joback Method
cpg	480.46	J/mol×K	578.62	Joback Method
cpg	551.11	J/mol×K	722.69	Joback Method
dvisc	0.0001764	Pa×s	549.81	Joback Method
dvisc	0.0002373	Pa×s	505.20	Joback Method
dvisc	0.0003381	Pa×s	460.59	Joback Method
dvisc	0.0005197	Pa×s	415.99	Joback Method
dvisc	0.0008857	Pa×s	371.38	Joback Method
dvisc	0.0017460	Pa×s	326.77	Joback Method
dvisc	0.0042661	Pa×s	282.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49620e+01
Coeff. B	-4.43474e+03
Coeff. C	-8.24710e+01
Temperature range (K), min.	384.68
Temperature range (K), max.	542.00

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56423439&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

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume