n-Valeric acid cis-3-hexenyl ester

Other names:	(3Z)-3-Hexenyl pentanoate
	(Z)-3-Hexen-1-ol, pentanoate
	(Z)-3-Hexenyl pentanoate
	(Z)-3-Hexenyl valerate
	(Z)-Hex-3-enyl valerate
	Pentanoic acid, (3Z)-3-hexen-1-yl ester
	Pentanoic acid, (3Z)-3-hexenyl ester
	Pentanoic acid, 3-hexenyl ester, (Z)-
	cis-3-Hexenyl N-valerate
	cis-3-Hexenyl valerate
Inchi:	InChI=1S/C11H20O2/c1-3-5-7-8-10-13-11(12)9-6-4-2/h5,7H,3-4,6,8-10H2,1-2H3/b7-5-
InchiKey:	XPFTVTFOOTVHIA-ALCCZGGFSA-N
Formula:	C11H20O2
SMILES:	CCC=CCCOC(=O)CCCC
Mol. weight [g/mol]:	184.28
CAS:	35852-46-1

Physical Properties

Property code	Value	Unit	Source
gf	-111.96	kJ/mol	Joback Method
hf	-397.95	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1235.80		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1235.80		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1518.00		NIST Webbook

ripol	1554.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1521.00		NIST Webbook
tb	531.53	K	Joback Method
tc	709.61	K	Joback Method
tf	280.81	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.35	J/mol×K	531.53	Joback Method
cpg	411.96	J/mol×K	561.21	Joback Method
cpg	425.95	J/mol×K	590.89	Joback Method
cpg	439.33	J/mol×K	620.57	Joback Method
cpg	452.12	J/mol×K	650.25	Joback Method
cpg	464.33	J/mol×K	679.93	Joback Method
cpg	475.98	J/mol×K	709.61	Joback Method
dvisc	0.0029775	Pa×s	280.81	Joback Method
dvisc	0.0013650	Pa×s	322.60	Joback Method
dvisc	0.0007484	Pa×s	364.38	Joback Method
dvisc	0.0004643	Pa×s	406.17	Joback Method
dvisc	0.0003149	Pa×s	447.96	Joback Method
dvisc	0.0002282	Pa×s	489.74	Joback Method
dvisc	0.0001740	Pa×s	531.53	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65377e+01
Coeff. B	-4.97929e+03
Coeff. C	-8.36470e+01
Temperature range (K), min.	390.06
Temperature range (K), max.	527.19

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35852461&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

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