Pentanoic acid, pentyl ester

Other names:	1-Pentyl n-valerate
	Amyl valerate
	Amyl valerianate
	NSC 76414
	Pentyl ester of pentanoic acid
	Pentyl pentanoate
	Pentyl valerate
	Valeric acid, pentyl ester
	n-Amyl n-valerate
	n-Pentyl valerate
Inchi:	InChI=1S/C10H20O2/c1-3-5-7-9-12-10(11)8-6-4-2/h3-9H2,1-2H3
InchiKey:	FGPPDYNPZTUNIU-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCOC(=O)CCCC
Mol. weight [g/mol]:	172.26
CAS:	2173-56-0

Physical Properties

Property code	Value	Unit	Source
gf	-200.60	kJ/mol	Joback Method
hf	-494.53	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	47.01	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.910		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1173.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1185.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1155.00		NIST Webbook

rinpol	1170.00		NIST Webbook
rinpol	1188.00		NIST Webbook
ripol	1406.00		NIST Webbook
ripol	1401.00		NIST Webbook
ripol	1401.00		NIST Webbook
ripol	1401.00		NIST Webbook
ripol	1406.00		NIST Webbook
tb	479.00 ± 4.00	K	NIST Webbook
tb	476.90 ± 2.00	K	NIST Webbook
tc	676.79	K	Joback Method
tf	274.62	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.11	J/mol×K	504.49	Joback Method
cpg	382.26	J/mol×K	533.21	Joback Method
cpg	395.89	J/mol×K	561.92	Joback Method
cpg	409.00	J/mol×K	590.64	Joback Method
cpg	421.59	J/mol×K	619.36	Joback Method
cpg	433.67	J/mol×K	648.08	Joback Method
cpg	445.25	J/mol×K	676.79	Joback Method
dvisc	0.0032806	Pa×s	274.62	Joback Method
dvisc	0.0015931	Pa×s	312.93	Joback Method
dvisc	0.0009057	Pa×s	351.24	Joback Method
dvisc	0.0005753	Pa×s	389.56	Joback Method
dvisc	0.0003964	Pa×s	427.87	Joback Method
dvisc	0.0002904	Pa×s	466.18	Joback Method
dvisc	0.0002230	Pa×s	504.49	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48510e+01
Coeff. B	-4.14716e+03

Coeff. C	-7.37140e+01
Temperature range (K), min.	358.48
Temperature range (K), max.	508.45

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2173560&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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1120.mol
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume