Pentanoic acid, heptyl ester

Other names:	39840N
	ENT 30517
	Heptyl pentanoate
	Heptyl valerate
	Valeric acid, heptyl ester
Inchi:	InChI=1S/C12H24O2/c1-3-5-7-8-9-11-14-12(13)10-6-4-2/h3-11H2,1-2H3
InchiKey:	YJARPRLGQQFGOI-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCCOC(=O)CCCC
Mol. weight [g/mol]:	200.32
CAS:	5451-80-9

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	1372.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1376.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1614.00		NIST Webbook
tb	516.80 ± 2.00	K	NIST Webbook
tb	518.36 ± 0.30	K	NIST Webbook
tc	720.05	K	Joback Method
tf	226.80 ± 0.50	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	479.84	J/mol×K	578.55	Joback Method
cpg	494.90	J/mol×K	606.85	Joback Method
cpg	509.36	J/mol×K	635.15	Joback Method
cpg	523.23	J/mol×K	663.45	Joback Method
cpg	536.51	J/mol×K	691.75	Joback Method
cpg	549.22	J/mol×K	720.05	Joback Method
dvisc	0.0030867	Pa×s	297.16	Joback Method
dvisc	0.0014485	Pa×s	339.34	Joback Method
dvisc	0.0008035	Pa×s	381.52	Joback Method
dvisc	0.0005012	Pa×s	423.70	Joback Method
dvisc	0.0003406	Pa×s	465.89	Joback Method
dvisc	0.0002467	Pa×s	508.07	Joback Method
dvisc	0.0001878	Pa×s	550.25	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50742e+01
Coeff. B	-4.53104e+03
Coeff. C	-8.52510e+01
Temperature range (K), min.	391.68
Temperature range (K), max.	549.37

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5451809&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/mol1129.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