Propanoic acid, heptyl ester

Other names:	ENT 21504
	Heptyl propanoate
	Heptyl propionate
	Propionic acid, heptyl ester
	n-Heptyl propionate
Inchi:	InChI=1S/C10H20O2/c1-3-5-6-7-8-9-12-10(11)4-2/h3-9H2,1-2H3
InchiKey:	BGYICJVBGZQOCY-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCCCOC(=O)CC
Mol. weight [g/mol]:	172.26
CAS:	2216-81-1

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	1202.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1181.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1178.00		NIST Webbook
rinpol	1201.11		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1180.06		NIST Webbook

rinpol	1182.00		NIST Webbook
ripol	1427.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1444.07		NIST Webbook
ripol	1446.66		NIST Webbook
ripol	1445.70		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1461.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1460.00		NIST Webbook
ripol	1447.76		NIST Webbook
tb	483.19 ± 0.30	K	NIST Webbook
tb	481.20 ± 2.00	K	NIST Webbook
tc	676.79	K	Joback Method
tf	222.30 ± 0.50	K	NIST Webbook
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	433.67	J/mol×K	648.08	Joback Method
cpg	421.59	J/mol×K	619.36	Joback Method
cpg	409.00	J/mol×K	590.64	Joback Method
cpg	395.89	J/mol×K	561.92	Joback Method
cpg	382.26	J/mol×K	533.21	Joback Method
cpg	445.25	J/mol×K	676.79	Joback Method
dvisc	0.0002230	Pa×s	504.49	Joback Method
dvisc	0.0002904	Pa×s	466.18	Joback Method
dvisc	0.0003964	Pa×s	427.87	Joback Method
dvisc	0.0005753	Pa×s	389.56	Joback Method
dvisc	0.0009057	Pa×s	351.24	Joback Method
dvisc	0.0015931	Pa×s	312.93	Joback Method
dvisc	0.0032806	Pa×s	274.62	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51545e+01
Coeff. B	-4.29586e+03
Coeff. C	-7.54660e+01
Temperature range (K), min.	364.42
Temperature range (K), max.	511.90

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1123.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2216811&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