Butanoic acid, heptyl ester

Other names:	Butyric acid, heptyl ester
	Heptyl butanoate
	Heptyl butyrate
	n-Heptyl butanoate
	n-Heptyl n-butyrate
Inchi:	InChI=1S/C11H22O2/c1-3-5-6-7-8-10-13-11(12)9-4-2/h3-10H2,1-2H3
InchiKey:	JPQHLIYIQARLQM-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CCCCCCCOC(=O)CCC
Mol. weight [g/mol]:	186.29
CAS:	5870-93-9

Physical Properties

Property code	Value	Unit	Source
gf	-192.18	kJ/mol	Joback Method
hf	-515.17	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.300		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	1287.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1274.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1502.00		NIST Webbook

ripol	1520.00		NIST Webbook
ripol	1503.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1526.00		NIST Webbook
tb	499.02 ± 0.30	K	NIST Webbook
tb	498.40 ± 1.50	K	NIST Webbook
tc	698.36	K	Joback Method
tf	215.70 ± 0.50	K	NIST Webbook
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.39	J/mol×K	669.86	Joback Method
cpg	496.57	J/mol×K	698.36	Joback Method
cpg	415.24	J/mol×K	527.37	Joback Method
cpg	430.19	J/mol×K	555.87	Joback Method
cpg	444.58	J/mol×K	584.37	Joback Method
cpg	458.41	J/mol×K	612.87	Joback Method
cpg	471.67	J/mol×K	641.36	Joback Method
dvisc	0.0002056	Pa×s	527.37	Joback Method
dvisc	0.0002689	Pa×s	487.12	Joback Method
dvisc	0.0032030	Pa×s	285.89	Joback Method
dvisc	0.0015281	Pa×s	326.14	Joback Method
dvisc	0.0008577	Pa×s	366.38	Joback Method
dvisc	0.0005398	Pa×s	406.63	Joback Method
dvisc	0.0003692	Pa×s	446.88	Joback Method
hvapt	58.70	kJ/mol	441.00	NIST Webbook
hvapt	65.10	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55310e+01
Coeff. B	-4.51825e+03
Coeff. C	-7.99140e+01
Temperature range (K), min.	376.32
Temperature range (K), max.	522.03

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5870939&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
Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.015

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
hvapt:	Enthalpy of vaporization at a given temperature
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