HEXADECANOIC ACID, BUTYL ESTER

Other names:	Butyl ester of hexadecanoic acid
	Butyl hexadecanoate
	Butyl palmitate
	Palmitic acid, butyl ester
	n-Butyl hexadecanoate
	n-Butyl palmitate
Inchi:	InChI=1S/C20H40O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-20(21)22-19-6-4-2/h3-19
InchiKey:	GLYJVQDYLFAUFC-UHFFFAOYSA-N
Formula:	C20H40O2
SMILES:	CCCCCCCCCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	312.54
CAS:	111-06-8

Physical Properties

Property code	Value	Unit	Source
af	0.9747		Cheméo Relay (1.0)
hf	-774.12	kJ/mol	Cheméo Relay (1.0)
hfus	50.34	kJ/mol	Joback Method
hvap	98.26	kJ/mol	Cheméo Relay (1.0)
ie	9.69	eV	Cheméo Relay (1.0)
log10ws	-6.82		Cheméo Relay (1.0)
logp	6.811		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2188.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2188.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
ripol	2419.00		NIST Webbook
tb	592.59	K	Cheméo Relay (1.0)
tc	773.35	K	Cheméo Relay (1.0)
tf	287.72	K	Cheméo Relay (1.0)
vc	1.182	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.52	J/mol×K	733.29	Joback Method
cpg	1013.17	J/mol×K	904.52	Joback Method
cpg	997.86	J/mol×K	875.99	Joback Method
cpg	981.74	J/mol×K	847.45	Joback Method
cpg	964.76	J/mol×K	818.91	Joback Method
cpg	946.91	J/mol×K	790.37	Joback Method
cpg	928.17	J/mol×K	761.83	Joback Method
dvisc	0.0002156	Pa×s	560.31	Joback Method
dvisc	0.0000733	Pa×s	733.29	Joback Method
dvisc	0.0000988	Pa×s	675.63	Joback Method
dvisc	0.0001407	Pa×s	617.97	Joback Method
dvisc	0.0016619	Pa×s	387.32	Joback Method
dvisc	0.0003644	Pa×s	502.64	Joback Method
dvisc	0.0007053	Pa×s	444.98	Joback Method
hvapt	93.80	kJ/mol	368.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.02510e+01
Coeff. B	-7.76715e+03
Coeff. C	-1.28730e+02
Temperature range (K), min.	517.80
Temperature range (K), max.	648.64

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C111068&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
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