Butyric acid, hexadecyl ester

Other names:	Butanoic acid, hexadecyl ester
	Hexadecyl butyrate
Inchi:	InChI=1S/C20H40O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-19-22-20(21)18-4-2/h3-19
InchiKey:	NJVKAQGGBANCKG-UHFFFAOYSA-N
Formula:	C20H40O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCC
Mol. weight [g/mol]:	312.53
CAS:	6221-99-4

Physical Properties

Property code	Value	Unit	Source
gf	-116.40	kJ/mol	Joback Method
hf	-700.93	kJ/mol	Joback Method
hfus	50.34	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.811		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2172.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2154.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2164.00		NIST Webbook
rinpol	2169.00		NIST Webbook
ripol	2400.00		NIST Webbook
tb	733.29	K	Joback Method
tc	904.52	K	Joback Method
tf	278.00 ± 4.00	K	NIST Webbook
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.52	J/mol×K	733.29	Joback Method
cpg	928.17	J/mol×K	761.83	Joback Method
cpg	946.91	J/mol×K	790.37	Joback Method
cpg	964.76	J/mol×K	818.91	Joback Method
cpg	981.74	J/mol×K	847.45	Joback Method
cpg	997.86	J/mol×K	875.99	Joback Method
cpg	1013.17	J/mol×K	904.52	Joback Method
dvisc	0.0016619	Pa×s	387.32	Joback Method
dvisc	0.0007053	Pa×s	444.98	Joback Method
dvisc	0.0003644	Pa×s	502.64	Joback Method
dvisc	0.0002156	Pa×s	560.30	Joback Method
dvisc	0.0001407	Pa×s	617.97	Joback Method
dvisc	0.0000988	Pa×s	675.63	Joback Method
dvisc	0.0000733	Pa×s	733.29	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C6221994&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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