Pentadecanoic acid, butyl ester

Other names: Butyl pentadecanoate
Inchi: InChI=1S/C19H38O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19(20)21-18-6-4-2/h3-18H2
InchiKey: KRMLKIYWYMUWHP-UHFFFAOYSA-N
Formula: C19H38O2
SMILES: CCCCCCCCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]: 298.50
CAS: 35996-97-5

Physical Properties

Property code	Value	Unit	Source
gf	-124.82	kJ/mol	Joback Method
hf	-680.29	kJ/mol	Joback Method
hfus	47.75	kJ/mol	Joback Method
hvap	67.04	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.421		Crippen Method
mcvol	286.010	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
ripol	2330.00		NIST Webbook
ripol	2330.00		NIST Webbook
tb	710.41	K	Joback Method
tc	879.90	K	Joback Method
tf	376.05	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.69	J/mol×K	710.41	Joback Method
cpg	867.91	J/mol×K	738.66	Joback Method
cpg	886.25	J/mol×K	766.91	Joback Method

cpg	903.75	J/mol×K	795.15	Joback Method
cpg	920.41	J/mol×K	823.40	Joback Method
cpg	936.27	J/mol×K	851.65	Joback Method
cpg	951.34	J/mol×K	879.90	Joback Method
dvisc	0.0018384	Pa×s	376.05	Joback Method
dvisc	0.0007881	Pa×s	431.78	Joback Method
dvisc	0.0004101	Pa×s	487.50	Joback Method
dvisc	0.0002440	Pa×s	543.23	Joback Method
dvisc	0.0001599	Pa×s	598.96	Joback Method
dvisc	0.0001126	Pa×s	654.68	Joback Method
dvisc	0.0000838	Pa×s	710.41	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35996975&Units=SI

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