10-Undecenoic acid, butyl ester

Other names:	Butyl 10-undecenoate
	Butyl 10-undecylenate
	Butyl undecylenate
	butyl undec-10-enoate
	n-Butyl 10-undecenoate
Inchi:	InChI=1S/C15H28O2/c1-3-5-7-8-9-10-11-12-13-15(16)17-14-6-4-2/h3H,1,4-14H2,2H3
InchiKey:	GRAORJFMGCQWRN-UHFFFAOYSA-N
Formula:	C15H28O2
SMILES:	C=CCCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	240.38
CAS:	109-42-2

Physical Properties

Property code	Value	Unit	Source
gf	-70.66	kJ/mol	Joback Method
hf	-472.30	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.636		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1972.00		NIST Webbook
ripol	1972.00		NIST Webbook
tb	615.57	K	Joback Method
tc	785.30	K	Joback Method
tf	329.21	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.68	J/mol×K	615.57	Joback Method
cpg	676.23	J/mol×K	757.01	Joback Method
cpg	662.10	J/mol×K	728.72	Joback Method
cpg	647.30	J/mol×K	700.44	Joback Method
cpg	631.81	J/mol×K	672.15	Joback Method
cpg	615.61	J/mol×K	643.86	Joback Method
cpg	689.70	J/mol×K	785.30	Joback Method
dvisc	0.0001429	Pa×s	615.57	Joback Method
dvisc	0.0001884	Pa×s	567.84	Joback Method
dvisc	0.0002614	Pa×s	520.12	Joback Method
dvisc	0.0003874	Pa×s	472.39	Joback Method
dvisc	0.0006273	Pa×s	424.66	Joback Method
dvisc	0.0011478	Pa×s	376.94	Joback Method
dvisc	0.0025018	Pa×s	329.21	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40739e+01
Coeff. B	-4.47262e+03
Coeff. C	-9.32380e+01
Temperature range (K), min.	417.66
Temperature range (K), max.	603.67

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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