BUTYL DODECANOATE(LAURATE)

Other names:	Lauric acid butyl ester
	Lauric acid n-butyl ester
	butyl dodecanoate
	butyl laurate
	dodecanoic acid, butyl ester
	lauric acid, butyl ester
	n-Butyl n-dodecanoate
	n-butyl laurate
Inchi:	InChI=1S/C16H32O2/c1-3-5-7-8-9-10-11-12-13-14-16(17)18-15-6-4-2/h3-15H2,1-2H3
InchiKey:	NDKYEUQMPZIGFN-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCCCCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	256.43
CAS:	106-18-3

Physical Properties

Property code	Value	Unit	Source
af	0.8342		Cheméo Relay (1.0)
hf	-692.64	kJ/mol	Cheméo Relay (1.0)
hfus	39.98	kJ/mol	Joback Method
hvap	89.20	kJ/mol	NIST Webbook
ie	9.57	eV	Cheméo Relay (1.0)
log10ws	-5.44		Cheméo Relay (1.0)
logp	5.251		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1772.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1786.00		NIST Webbook
rinpol	1786.00		NIST Webbook
ripol	2035.00		NIST Webbook
ripol	2000.00		NIST Webbook
ripol	2035.00		NIST Webbook
ripol	2024.00		NIST Webbook

tb	560.94	K	Cheméo Relay (1.0)
tc	737.88	K	Cheméo Relay (1.0)
tf	266.31 ± 0.20	K	NIST Webbook
vc	0.954	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.90	J/mol×K	781.24	Joback Method
cpg	772.16	J/mol×K	809.14	Joback Method
cpg	693.74	J/mol×K	669.66	Joback Method
cpg	710.87	J/mol×K	697.56	Joback Method
cpg	727.27	J/mol×K	725.45	Joback Method
cpg	742.94	J/mol×K	753.35	Joback Method
cpg	675.85	J/mol×K	641.77	Joback Method
dvisc	0.0005682	Pa×s	442.08	Joback Method
dvisc	0.0010661	Pa×s	392.16	Joback Method
dvisc	0.0024033	Pa×s	342.24	Joback Method
dvisc	0.0003441	Pa×s	492.00	Joback Method
dvisc	0.0002286	Pa×s	541.93	Joback Method
dvisc	0.0001627	Pa×s	591.85	Joback Method
dvisc	0.0001221	Pa×s	641.77	Joback Method
hvapt	75.80	kJ/mol	363.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49106e+01
Coeff. B	-4.87568e+03
Coeff. C	-9.90960e+01
Temperature range (K), min.	432.52
Temperature range (K), max.	607.02

Sources

Solubilities of n-Butyl Esters in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je500309x
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106183&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0, beta):	
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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