Butyl caprylate

Other names:	Butyl octanoate
	Caprylic acid n-butyl ester
	Octanoic acid, butyl ester
	n-Butyl n-octanoate
	n-Butyl octanoate
	n-Butylcaprylate
	n-Caprylic acid n-butyl ester
Inchi:	InChI=1S/C12H24O2/c1-3-5-7-8-9-10-12(13)14-11-6-4-2/h3-11H2,1-2H3
InchiKey:	PSXNDMJWRZYVTM-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	200.32
CAS:	589-75-3

Physical Properties

Property code	Value	Unit	Source
gf	-183.76	kJ/mol	Joback Method
hf	-535.81	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	51.46	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.690		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1388.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1370.00		NIST Webbook

rinpol	1374.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1370.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1619.00		NIST Webbook
tb	518.17 ± 0.30	K	NIST Webbook
tb	513.70 ± 2.00	K	NIST Webbook
tc	720.05	K	Joback Method
tf	230.30 ± 0.50	K	NIST Webbook
tf	230.20 ± 0.80	K	NIST Webbook
tt	230.00	K	Heat capacities of potential organic phase change materials
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.17	J/mol×K	550.25	Joback Method
cpg	479.84	J/mol×K	578.55	Joback Method
cpg	494.90	J/mol×K	606.85	Joback Method
cpg	509.36	J/mol×K	635.15	Joback Method
cpg	523.23	J/mol×K	663.45	Joback Method
cpg	536.51	J/mol×K	691.75	Joback Method
cpg	549.22	J/mol×K	720.05	Joback Method

dvisc	0.0030867	Pa×s	297.16	Joback Method
dvisc	0.0014485	Pa×s	339.34	Joback Method
dvisc	0.0008035	Pa×s	381.52	Joback Method
dvisc	0.0005012	Pa×s	423.70	Joback Method
dvisc	0.0003406	Pa×s	465.89	Joback Method
dvisc	0.0002467	Pa×s	508.07	Joback Method
dvisc	0.0001878	Pa×s	550.25	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47253e+01
Coeff. B	-4.38871e+03
Coeff. C	-8.39450e+01
Temperature range (K), min.	387.92
Temperature range (K), max.	550.14

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Heat capacities of potential organic phase change materials: https://www.doi.org/10.1016/j.jct.2018.08.014

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=C589753&Units=SI

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

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
tt:	Triple Point Temperature
vc:	Critical Volume