Nonanoic acid, butyl ester

Other names:	Butyl nonanoate
	Butyl pelargonate
	butyl nonan-1-oate
	n-Butyl nonanoate
	n-Pelargonic acid, butyl ester
Inchi:	InChI=1S/C13H26O2/c1-3-5-7-8-9-10-11-13(14)15-12-6-4-2/h3-12H2,1-2H3
InchiKey:	DOLFPCDDMUMIMR-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	214.34
CAS:	50623-57-9

Physical Properties

Property code	Value	Unit	Source
gf	-175.34	kJ/mol	Joback Method
hf	-556.45	kJ/mol	Joback Method
hfus	32.21	kJ/mol	Joback Method
hvap	53.69	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.080		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
ripol	1725.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1700.00		NIST Webbook
tb	573.13	K	Joback Method
tc	741.92	K	Joback Method
tf	235.20 ± 0.70	K	NIST Webbook
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.80	J/mol×K	573.13	Joback Method
cpg	531.11	J/mol×K	601.26	Joback Method
cpg	546.77	J/mol×K	629.39	Joback Method
cpg	561.79	J/mol×K	657.52	Joback Method
cpg	576.19	J/mol×K	685.66	Joback Method
cpg	589.97	J/mol×K	713.79	Joback Method
cpg	603.14	J/mol×K	741.92	Joback Method
dvisc	0.0029408	Pa×s	308.43	Joback Method
dvisc	0.0013589	Pa×s	352.55	Joback Method
dvisc	0.0007456	Pa×s	396.66	Joback Method
dvisc	0.0004613	Pa×s	440.78	Joback Method
dvisc	0.0003115	Pa×s	484.90	Joback Method
dvisc	0.0002245	Pa×s	529.01	Joback Method
dvisc	0.0001702	Pa×s	573.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55660e+01
Coeff. B	-4.79858e+03
Coeff. C	-8.93240e+01
Temperature range (K), min.	403.40
Temperature range (K), max.	557.27

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.26763e+02
Coeff. B	-1.29847e+04
Coeff. C	-1.57230e+01
Coeff. D	5.80566e-06
Temperature range (K), min.	235.15

Temperature range (K), max.	652.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50623579&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1132
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1132.mol
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

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