Butanoic acid, anhydride

Other names:	Anhydrid kyseliny maselne
	BUTANOIC ANHYDRIDE
	BUTYRYL OXIDE
	Butanoic acid, 1,1'-anhydride
	Butyranhydrid
	Butyric acid anhydride
	Butyric anhydride
	N-BUTYRIC ACID ANHYDRIDE
	UN 2739
	n-Butanoic anhydride
	n-Butyric anhydride
Inchi:	InChI=1S/C8H14O3/c1-3-5-7(9)11-8(10)6-4-2/h3-6H2,1-2H3
InchiKey:	YHASWHZGWUONAO-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	CCCC(=O)OC(=O)CCC
Mol. weight [g/mol]:	158.19
CAS:	106-31-0

Physical Properties

Property code	Value	Unit	Source
gf	-346.36	kJ/mol	Joback Method
hf	-565.83	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	49.30	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.656		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=1)		KDB
nfpas	%!d(float64=1)		KDB
pc	2838.39	kPa	Joback Method
tb	471.40 ± 0.60	K	NIST Webbook
tb	464.15 ± 2.50	K	NIST Webbook
tb	471.35 ± 0.50	K	NIST Webbook
tb	471.00 ± 0.50	K	NIST Webbook
tc	697.35	K	Joback Method
tf	198.15 ± 0.60	K	NIST Webbook

vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.67	J/mol×K	512.60	Joback Method
cpg	310.25	J/mol×K	543.39	Joback Method
cpg	321.37	J/mol×K	574.18	Joback Method
cpg	332.03	J/mol×K	604.98	Joback Method
cpg	342.23	J/mol×K	635.77	Joback Method
cpg	351.97	J/mol×K	666.56	Joback Method
cpg	361.25	J/mol×K	697.35	Joback Method
dvisc	0.0027356	Pa×s	302.01	Joback Method
dvisc	0.0015339	Pa×s	337.11	Joback Method
dvisc	0.0009592	Pa×s	372.21	Joback Method
dvisc	0.0006504	Pa×s	407.31	Joback Method
dvisc	0.0004690	Pa×s	442.40	Joback Method
dvisc	0.0003549	Pa×s	477.50	Joback Method
dvisc	0.0002790	Pa×s	512.60	Joback Method
hvapt	49.10	kJ/mol	409.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	471.70	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64793e+01
Coeff. B	-5.44987e+03
Coeff. C	-1.19200e+01
Temperature range (K), min.	348.50

Temperature range (K), max.	499.92

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.82855e+02
Coeff. B	-1.39777e+04
Coeff. C	-2.46850e+01
Coeff. D	1.56521e-05
Temperature range (K), min.	199.85
Temperature range (K), max.	639.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106310&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=993
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/mol993.mol

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating

nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume