Propanoic acid, anhydride

Other names:	Anhydrid kyseliny propionove C2H5C(O)OC(O)C2H5 METHYLACETIC ANHYDRIDE PROPIONIC ACID ANHYDRIDE PROPIONYL OXIDE Propanoic acid, 1,1'-anhydride Propanoic anhydride Propionic anhydride UN 2496 propionic acid, anhydride
Inchi:	InChI=1S/C6H10O3/c1-3-5(7)9-6(8)4-2/h3-4H2,1-2H3
InchiKey:	WYVAMUWZEOHJOQ-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CCC(=O)OC(=O)CC
Mol. weight [g/mol]:	130.14
CAS:	123-62-6

Physical Properties

Property code	Value	Unit	Source
gf	-363.20	kJ/mol	Joback Method
hf	-524.55	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	44.85	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.876		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
nfpas	%!d(float64=1)		KDB
pc	3522.09	kPa	Joback Method
tb	442.15	K	NIST Webbook
tb	440.15 ± 1.50	K	NIST Webbook
tb	440.15	K	KDB
tb	440.20	K	NIST Webbook
tb	438.15 ± 3.00	K	NIST Webbook
tb	440.40 ± 0.50	K	NIST Webbook
tb	440.00 ± 0.50	K	NIST Webbook

tb	438.15 ± 2.00	K	NIST Webbook
tb	469.15 ± 1.00	K	NIST Webbook
tc	655.65	K	Joback Method
tf	228.15 ± 0.50	K	NIST Webbook
tf	230.15	K	NIST Webbook
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.00	J/mol×K	466.84	Joback Method
cpg	224.34	J/mol×K	498.31	Joback Method
cpg	233.35	J/mol×K	529.78	Joback Method
cpg	242.00	J/mol×K	561.25	Joback Method
cpg	250.31	J/mol×K	592.71	Joback Method
cpg	258.27	J/mol×K	624.18	Joback Method
cpg	265.88	J/mol×K	655.65	Joback Method
dvisc	0.0015646	Pa×s	310.70	Joback Method
dvisc	0.0026736	Pa×s	279.47	Joback Method
dvisc	0.0010097	Pa×s	341.93	Joback Method
dvisc	0.0007012	Pa×s	373.16	Joback Method
dvisc	0.0005151	Pa×s	404.38	Joback Method
dvisc	0.0003956	Pa×s	435.61	Joback Method
dvisc	0.0003147	Pa×s	466.84	Joback Method
hvapt	48.20	kJ/mol	366.50	NIST Webbook
hvapt	52.20	kJ/mol	390.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	340.70	K	2.40	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.40259e+01
Coeff. B	-1.62754e+04
Coeff. C	3.98458e+02
Temperature range (K), min.	287.16
Temperature range (K), max.	471.21

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.33844e+01
Coeff. B	-8.86827e+03
Coeff. C	-9.79008e+00
Coeff. D	4.94606e-06
Temperature range (K), min.	228.15
Temperature range (K), max.	618.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123626&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=991
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Experimental Determination and Modeling of the Phase Behavior of the CO2 + Propionic Anhydride Binary System at High Pressure:	https://www.doi.org/10.1021/acs.jced.6b00595
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol991.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