Hexanoic acid, anhydride

Other names:	Caproic acid anhydride
	Caproic anhydride
	Capronic acid anhydride
	Capronic anhydride
	Hexanoic acid, 1,1'-anhydride
	Hexanoic anhydride
	Hexanoyl anhydride
	n-Caproic anhydride
	n-Hexanoic acid anhydride
	n-Hexanoic anhydride
Inchi:	InChI=1S/C12H22O3/c1-3-5-7-9-11(13)15-12(14)10-8-6-4-2/h3-10H2,1-2H3
InchiKey:	PKHMTIRCAFTBDS-UHFFFAOYSA-N
Formula:	C12H22O3
SMILES:	CCCCCC(=O)OC(=O)CCCCC
Mol. weight [g/mol]:	214.30
CAS:	2051-49-2

Physical Properties

Property code	Value	Unit	Source
gf	-312.68	kJ/mol	Joback Method
hf	-648.39	kJ/mol	Joback Method
hfus	31.22	kJ/mol	Joback Method
hvap	58.21	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.217		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
tb	520.20	K	NIST Webbook
tb	512.15 ± 2.00	K	NIST Webbook
tc	781.95	K	Joback Method
tf	347.09	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.63	J/mol×K	781.95	Joback Method
cpg	488.75	J/mol×K	604.12	Joback Method
cpg	503.49	J/mol×K	633.76	Joback Method
cpg	517.57	J/mol×K	663.40	Joback Method
cpg	531.02	J/mol×K	693.04	Joback Method
cpg	543.84	J/mol×K	722.67	Joback Method
cpg	556.04	J/mol×K	752.31	Joback Method
dvisc	0.0001937	Pa×s	604.12	Joback Method
dvisc	0.0024044	Pa×s	347.09	Joback Method
dvisc	0.0012547	Pa×s	389.93	Joback Method
dvisc	0.0007447	Pa×s	432.77	Joback Method
dvisc	0.0004856	Pa×s	475.61	Joback Method
dvisc	0.0003398	Pa×s	518.44	Joback Method
dvisc	0.0002511	Pa×s	561.28	Joback Method
rhol	923.96	kg/m3	298.15	Excess Molar Enthalpies of Binary Systems of n-Valeric Anhydride or n-Hexanoic Anhydride with n-Dodecane, n-Tetradecane, or n-Hexadecane at 298.15 K

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol995.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Excess Molar Enthalpies of Binary Systems of n-Valeric Anhydride or n-Hexanoic Anhydride with n-Dodecane, n-Tetradecane, or n-Hexadecane at 298.15 K:	https://www.doi.org/10.1021/je900598y

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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume