Heptanoic acid, anhydride

Other names:	Heptanoic anhydride
	n-Heptanoic acid anhydride
	Enanthic anhydride
	Heptanoyl anhydride
	Oenanthic anhydride
	n-Heptanoic anhydride
Inchi:	InChI=1S/C14H26O3/c1-3-5-7-9-11-13(15)17-14(16)12-10-8-6-4-2/h3-12H2,1-2H3
InchiKey:	DAPZDAPTZFJZTO-UHFFFAOYSA-N
Formula:	C14H26O3
SMILES:	CCCCCCC(=O)OC(=O)CCCCCC
Mol. weight [g/mol]:	242.35
CAS:	626-27-7

Physical Properties

Property code	Value	Unit	Source
gf	-295.84	kJ/mol	Joback Method
hf	-689.67	kJ/mol	Joback Method
hfus	36.40	kJ/mol	Joback Method
hvap	62.66	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.997		Crippen Method
mcvol	217.130	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	1675.80		NIST Webbook
tb	541.20	K	NIST Webbook
tb	530.00 ± 5.00	K	NIST Webbook
tc	825.72	K	Joback Method
tf	260.75 ± 0.50	K	NIST Webbook
tf	290.00 ± 3.00	K	NIST Webbook
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	593.47	J/mol×K	649.88	Joback Method
cpg	665.58	J/mol×K	796.41	Joback Method
cpg	652.55	J/mol×K	767.10	Joback Method
cpg	638.84	J/mol×K	737.80	Joback Method
cpg	624.43	J/mol×K	708.49	Joback Method
cpg	609.31	J/mol×K	679.19	Joback Method
cpg	677.93	J/mol×K	825.72	Joback Method
dvisc	0.0001547	Pa×s	649.88	Joback Method
dvisc	0.0002021	Pa×s	603.17	Joback Method
dvisc	0.0002762	Pa×s	556.46	Joback Method
dvisc	0.0003996	Pa×s	509.75	Joback Method
dvisc	0.0006228	Pa×s	463.05	Joback Method
dvisc	0.0010725	Pa×s	416.34	Joback Method
dvisc	0.0021187	Pa×s	369.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	437.20	K	1.70	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626277&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume