OCTANOIC ANHYDRIDE

Other names: Octanoic acid, anhydride
Octanoic anhydride
Inchi: InChI=1S/C16H30O3/c1-3-5-7-9-11-13-15(17)19-16(18)14-12-10-8-6-4-2/h3-14H2,1-2H3
InchiKey: RAFYDKXYXRZODZ-UHFFFAOYSA-N
Formula: C16H30O3
SMILES: CCCCCCCC(=O)OC(=O)CCCCCCC
Mol. weight [g/mol]: 270.41

Physical Properties

Property code	Value	Unit	Source
af	0.8895		Cheméo Relay (1.0)
gf	-279.00	kJ/mol	Joback Method
hf	-860.49	kJ/mol	Cheméo Relay (1.0)
hfus	41.58	kJ/mol	Joback Method
hvap	77.75	kJ/mol	Cheméo Relay (1.0)
ie	9.79	eV	Cheméo Relay (1.0)
log10ws	-4.99		Cheméo Relay (1.0)
logp	4.777		Crippen Method
mcvol	245.310	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	1878.30		NIST Webbook
tb	555.70	K	NIST Webbook
tc	741.47	K	Cheméo Relay (1.0)
tf	266.23	K	Cheméo Relay (1.0)
vc	0.954	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.61	J/mol×K	695.64	Joback Method
cpg	792.58	J/mol×K	871.01	Joback Method
cpg	779.64	J/mol×K	841.78	Joback Method
cpg	765.96	J/mol×K	812.55	Joback Method
cpg	751.54	J/mol×K	783.32	Joback Method

cpg	736.35	J/mol×K	754.10	Joback Method
cpg	720.38	J/mol×K	724.87	Joback Method
dvisc	0.0003211	Pa×s	543.90	Joback Method
dvisc	0.0001211	Pa×s	695.64	Joback Method
dvisc	0.0001593	Pa×s	645.06	Joback Method
dvisc	0.0002195	Pa×s	594.48	Joback Method
dvisc	0.0018108	Pa×s	392.17	Joback Method
dvisc	0.0005078	Pa×s	493.33	Joback Method
dvisc	0.0008918	Pa×s	442.75	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	459.20	K	2.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C623665&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

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

ie: Ionization energy

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