PROPANOIC ACID, NONYL ESTER

Other names: Nonyl propionate
Propionic acid nonyl ester
Inchi: InChI=1S/C12H24O2/c1-3-5-6-7-8-9-10-11-14-12(13)4-2/h3-11H2,1-2H3
InchiKey: MPSVBCFDONBQFM-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CCCCCCCCCOC(=O)CC
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
af	0.6890		Cheméo Relay (1.0)
gf	-183.76	kJ/mol	Joback Method
hf	-607.99	kJ/mol	Cheméo Relay (1.0)
hfus	29.62	kJ/mol	Joback Method
hvap	64.10	kJ/mol	Cheméo Relay (1.0)
ie	9.58	eV	Cheméo Relay (1.0)
log10ws	-4.02		Cheméo Relay (1.0)
logp	3.690		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1369.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1383.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1380.10		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1401.13		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1366.00		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1652.00		NIST Webbook
ripol	1680.00		NIST Webbook

ripol	1637.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1634.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1618.00		NIST Webbook
tb	507.39	K	Cheméo Relay (1.0)
tc	685.15	K	Cheméo Relay (1.0)
tf	246.01	K	Cheméo Relay (1.0)
vc	0.730	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.17	J/mol×K	550.25	Joback Method
cpg	479.84	J/mol×K	578.55	Joback Method
cpg	494.90	J/mol×K	606.85	Joback Method
cpg	509.36	J/mol×K	635.15	Joback Method
cpg	523.23	J/mol×K	663.45	Joback Method
cpg	536.51	J/mol×K	691.75	Joback Method
cpg	549.22	J/mol×K	720.05	Joback Method
dvisc	0.0030867	Pa×s	297.16	Joback Method
dvisc	0.0014485	Pa×s	339.34	Joback Method
dvisc	0.0008035	Pa×s	381.52	Joback Method
dvisc	0.0005012	Pa×s	423.70	Joback Method
dvisc	0.0003406	Pa×s	465.89	Joback Method
dvisc	0.0002467	Pa×s	508.07	Joback Method
dvisc	0.0001878	Pa×s	550.25	Joback Method

Sources

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

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

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):

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume