PROPANOIC ACID, 2-METHYL-, NONYL ESTER

Inchi: InChI=1S/C13H26O2/c1-4-5-6-7-8-9-10-11-15-13(14)12(2)3/h12H,4-11H2,1-3H3
InchiKey: SXMUYNHMPAZLEB-UHFFFAOYSA-N
Formula: C13H26O2
SMILES: CCCCCCCCCOC(=O)C(C)C
Mol. weight [g/mol]: 214.35

Physical Properties

Property code	Value	Unit	Source
af	0.6947		Cheméo Relay (1.0)
hf	-631.18	kJ/mol	Cheméo Relay (1.0)
hfus	28.69	kJ/mol	Joback Method
hvap	63.63	kJ/mol	Cheméo Relay (1.0)
ie	9.57	eV	Cheméo Relay (1.0)
log10ws	-4.33		Cheméo Relay (1.0)
logp	3.936		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1426.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1426.00		NIST Webbook
tb	502.42	K	Cheméo Relay (1.0)
tc	683.14	K	Cheméo Relay (1.0)
tf	237.34	K	Cheméo Relay (1.0)
vc	0.781	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.10	J/mol×K	572.69	Joback Method
cpg	531.74	J/mol×K	601.30	Joback Method
cpg	547.70	J/mol×K	629.91	Joback Method
cpg	563.00	J/mol×K	658.53	Joback Method
cpg	577.64	J/mol×K	687.14	Joback Method

cpg	591.64	J/mol×K	715.75	Joback Method
cpg	605.00	J/mol×K	744.36	Joback Method
dvisc	0.0040106	Pa×s	293.43	Joback Method
dvisc	0.0016218	Pa×s	339.97	Joback Method
dvisc	0.0008156	Pa×s	386.52	Joback Method
dvisc	0.0004755	Pa×s	433.06	Joback Method
dvisc	0.0003078	Pa×s	479.60	Joback Method
dvisc	0.0002152	Pa×s	526.15	Joback Method
dvisc	0.0001594	Pa×s	572.69	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10522346&Units=SI

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

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume