pentanoic acid, undecyl ester

Inchi: InChI=1S/C16H32O2/c1-3-5-7-8-9-10-11-12-13-15-18-16(17)14-6-4-2/h3-15H2,1-2H3
InchiKey: MTTLTPIFXXBAIT-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CCCCCCCCCCCOC(=O)CCCC
Mol. weight [g/mol]: 256.43

Physical Properties

Property code	Value	Unit	Source
af	0.8357		Cheméo Relay (1.0)
gf	-150.08	kJ/mol	Joback Method
hf	-691.99	kJ/mol	Cheméo Relay (1.0)
hfus	39.98	kJ/mol	Joback Method
hvap	80.10	kJ/mol	Cheméo Relay (1.0)
ie	9.53	eV	Cheméo Relay (1.0)
log10ws	-5.43		Cheméo Relay (1.0)
logp	5.251		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
tb	560.63	K	Cheméo Relay (1.0)
tc	737.35	K	Cheméo Relay (1.0)
tf	260.93	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	675.85	J/mol×K	641.77	Joback Method
cpg	693.74	J/mol×K	669.66	Joback Method
cpg	710.87	J/mol×K	697.56	Joback Method
cpg	727.27	J/mol×K	725.45	Joback Method
cpg	742.94	J/mol×K	753.35	Joback Method
cpg	757.90	J/mol×K	781.24	Joback Method
cpg	772.16	J/mol×K	809.14	Joback Method
dvisc	0.0024033	Pa×s	342.24	Joback Method

dvisc	0.0010661	Pa×s	392.16	Joback Method
dvisc	0.0005682	Pa×s	442.08	Joback Method
dvisc	0.0003441	Pa×s	492.00	Joback Method
dvisc	0.0002286	Pa×s	541.93	Joback Method
dvisc	0.0001627	Pa×s	591.85	Joback Method
dvisc	0.0001221	Pa×s	641.77	Joback Method

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=C81186234&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume