Dodecyl propyl carbonate

Inchi: InChI=1S/C16H32O3/c1-3-5-6-7-8-9-10-11-12-13-15-19-16(17)18-14-4-2/h3-15H2,1-2H3
InchiKey: KRFCCBNARQVDNQ-UHFFFAOYSA-N
Formula: C16H32O3
SMILES: CCCCCCCCCCCCOC(=O)OCCC
Mol. weight [g/mol]: 272.42
CAS: 959272-51-6

Physical Properties

Property code	Value	Unit	Source
gf	-255.08	kJ/mol	Joback Method
hf	-750.59	kJ/mol	Joback Method
hfus	41.17	kJ/mol	Joback Method
hvap	62.78	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	5.470		Crippen Method
mcvol	249.610	ml/mol	McGowan Method
pc	1346.69	kPa	Joback Method
rinpol	1868.00		NIST Webbook
tb	664.19	K	Joback Method
tc	832.28	K	Joback Method
tf	364.47	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.72	J/mol×K	664.19	Joback Method
cpg	724.41	J/mol×K	692.20	Joback Method
cpg	741.34	J/mol×K	720.22	Joback Method
cpg	757.52	J/mol×K	748.23	Joback Method
cpg	772.96	J/mol×K	776.25	Joback Method
cpg	787.68	J/mol×K	804.26	Joback Method
cpg	801.67	J/mol×K	832.28	Joback Method
dvisc	0.0016436	Pa×s	364.47	Joback Method

dvisc	0.0007663	Pa×s	414.42	Joback Method
dvisc	0.0004210	Pa×s	464.38	Joback Method
dvisc	0.0002598	Pa×s	514.33	Joback Method
dvisc	0.0001747	Pa×s	564.28	Joback Method
dvisc	0.0001253	Pa×s	614.24	Joback Method
dvisc	0.0000944	Pa×s	664.19	Joback Method

Sources

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=C959272516&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume