DODECANOIC ACID, 12-HYDROXY-, METHYL ESTER

Inchi: InChI=1S/C13H26O3/c1-16-13(15)11-9-7-5-3-2-4-6-8-10-12-14/h14H,2-12H2,1H3
InchiKey: WVYBBOXJKXXXOY-UHFFFAOYSA-N
Formula: C13H26O3
SMILES: COC(=O)CCCCCCCCCCCO
Mol. weight [g/mol]: 230.35

Physical Properties

Property code	Value	Unit	Source
af	0.9423		Cheméo Relay (1.0)
hf	-771.76	kJ/mol	Cheméo Relay (1.0)
hfus	36.30	kJ/mol	Joback Method
hvap	105.28	kJ/mol	Cheméo Relay (1.0)
ie	9.79	eV	Cheméo Relay (1.0)
log10ws	-3.41		Cheméo Relay (1.0)
logp	3.053		Crippen Method
mcvol	207.340	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
tb	577.80	K	Cheméo Relay (1.0)
tc	761.94	K	Cheméo Relay (1.0)
tf	308.00 ± 3.00	K	NIST Webbook
vc	0.793	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.17	J/mol×K	665.31	Joback Method
cpg	659.59	J/mol×K	832.17	Joback Method
cpg	648.32	J/mol×K	804.36	Joback Method
cpg	636.47	J/mol×K	776.55	Joback Method
cpg	624.05	J/mol×K	748.74	Joback Method
cpg	611.03	J/mol×K	720.93	Joback Method
cpg	597.40	J/mol×K	693.12	Joback Method
dvisc	0.0002116	Pa×s	517.28	Joback Method
dvisc	0.0000446	Pa×s	665.31	Joback Method

dvisc	0.0000689	Pa×s	615.97	Joback Method
dvisc	0.0001150	Pa×s	566.62	Joback Method
dvisc	0.0035060	Pa×s	369.25	Joback Method
dvisc	0.0004429	Pa×s	467.94	Joback Method
dvisc	0.0011030	Pa×s	418.59	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71655362&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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