NONANOIC ACID, 9-HYDROXY-, METHYL ESTER

Other names: methyl 9-hydroxynonanoate
Inchi: InChI=1S/C10H20O3/c1-13-10(12)8-6-4-2-3-5-7-9-11/h11H,2-9H2,1H3
InchiKey: RIZOOQYPYGPBOC-UHFFFAOYSA-N
Formula: C10H20O3
SMILES: COC(=O)CCCCCCCCO
Mol. weight [g/mol]: 188.27

Physical Properties

Property code	Value	Unit	Source
af	0.8362		Cheméo Relay (1.0)
hf	-710.67	kJ/mol	Cheméo Relay (1.0)
hfus	28.53	kJ/mol	Joback Method
hvap	91.61	kJ/mol	Cheméo Relay (1.0)
ie	9.80	eV	Cheméo Relay (1.0)
log10ws	-2.02		Cheméo Relay (1.0)
logp	1.882		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	544.69	K	Cheméo Relay (1.0)
tc	728.88	K	Cheméo Relay (1.0)
tf	296.27	K	Cheméo Relay (1.0)
vc	0.626	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.51	J/mol×K	596.67	Joback Method
cpg	440.83	J/mol×K	624.50	Joback Method
cpg	452.65	J/mol×K	652.33	Joback Method
cpg	463.99	J/mol×K	680.16	Joback Method
cpg	474.85	J/mol×K	707.98	Joback Method
cpg	485.23	J/mol×K	735.81	Joback Method
cpg	495.14	J/mol×K	763.64	Joback Method
dvisc	0.0060280	Pa×s	335.44	Joback Method

dvisc	0.0019204	Pa×s	378.98	Joback Method
dvisc	0.0007745	Pa×s	422.52	Joback Method
dvisc	0.0003701	Pa×s	466.05	Joback Method
dvisc	0.0002006	Pa×s	509.59	Joback Method
dvisc	0.0001198	Pa×s	553.13	Joback Method
dvisc	0.0000771	Pa×s	596.67	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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34957738&Units=SI

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.