Ethyl nerolate

Inchi: InChI=1S/C10H20O2/c1-8(2)5-4-6-9(3)7-10(11)12/h8-9H,4-7H2,1-3H3,(H,11,12)
InchiKey: DGGBNSXAFVNQJU-UHFFFAOYSA-N
Formula: C10H20O2
SMILES: CC(C)CCCC(C)CC(=O)O
Mol. weight [g/mol]: 172.27

Physical Properties

Property code	Value	Unit	Source
af	0.7401		Cheméo Relay (1.0)
hf	-635.02	kJ/mol	Cheméo Relay (1.0)
hfus	20.30	kJ/mol	Joback Method
hvap	83.66	kJ/mol	Cheméo Relay (1.0)
ie	9.83	eV	Cheméo Relay (1.0)
log10ws	-2.97		Cheméo Relay (1.0)
logp	2.924		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	1359.00		NIST Webbook
rinpol	1359.00		NIST Webbook
ripol	2123.00		NIST Webbook
tb	508.88	K	Cheméo Relay (1.0)
tc	692.18	K	Cheméo Relay (1.0)
tf	278.34	K	Cheméo Relay (1.0)
vc	0.564	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.51	J/mol×K	573.37	Joback Method
cpg	473.04	J/mol×K	746.05	Joback Method
cpg	462.78	J/mol×K	717.27	Joback Method
cpg	452.00	J/mol×K	688.49	Joback Method
cpg	440.70	J/mol×K	659.71	Joback Method
cpg	428.87	J/mol×K	630.93	Joback Method

cpg	416.47	J/mol×K	602.15	Joback Method
dvisc	0.0006431	Pa×s	428.29	Joback Method
dvisc	0.0000919	Pa×s	573.37	Joback Method
dvisc	0.0001560	Pa×s	525.01	Joback Method
dvisc	0.0002948	Pa×s	476.65	Joback Method
dvisc	0.0330442	Pa×s	283.21	Joback Method
dvisc	0.0017116	Pa×s	379.93	Joback Method
dvisc	0.0060601	Pa×s	331.57	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=C5698271&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume