methyl 18-methylnonadecanoate

Inchi: InChI=1S/C21H42O2/c1-20(2)18-16-14-12-10-8-6-4-5-7-9-11-13-15-17-19-21(22)23-3/h2
InchiKey: IVHQIMJNEKWLSS-UHFFFAOYSA-N
Formula: C21H42O2
SMILES: COC(=O)CCCCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 326.56
CAS: 65301-91-9

Physical Properties

Property code	Value	Unit	Source
af	0.9655		Cheméo Relay (1.0)
gf	-110.42	kJ/mol	Joback Method
hf	-795.15	kJ/mol	Cheméo Relay (1.0)
hfus	49.41	kJ/mol	Joback Method
hvap	110.35	kJ/mol	Cheméo Relay (1.0)
ie	9.86	eV	Cheméo Relay (1.0)
log10ws	-7.40		Cheméo Relay (1.0)
logp	7.057		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
tb	596.86	K	Cheméo Relay (1.0)
tc	781.28	K	Cheméo Relay (1.0)
tf	311.08	K	Cheméo Relay (1.0)
vc	1.215	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.75	J/mol×K	755.73	Joback Method
cpg	1076.91	J/mol×K	930.28	Joback Method
cpg	1061.34	J/mol×K	901.19	Joback Method
cpg	1044.89	J/mol×K	872.09	Joback Method
cpg	1027.53	J/mol×K	843.00	Joback Method
cpg	1009.24	J/mol×K	813.91	Joback Method
cpg	989.99	J/mol×K	784.82	Joback Method

dvisc	0.0001889	Pa×s	569.66	Joback Method
dvisc	0.0000590	Pa×s	755.73	Joback Method
dvisc	0.0000811	Pa×s	693.71	Joback Method
dvisc	0.0001187	Pa×s	631.68	Joback Method
dvisc	0.0018724	Pa×s	383.59	Joback Method
dvisc	0.0003366	Pa×s	507.64	Joback Method
dvisc	0.0007045	Pa×s	445.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65301919&Units=SI
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):	

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