METHYL DECENOATE

Other names: Methyl decenoate
Inchi: InChI=1S/C13H24O2/c1-3-4-5-6-7-8-9-10-11-12-13(14)15-2/h3H,1,4-12H2,2H3
InchiKey: ZIPHBQHTAWKZCG-UHFFFAOYSA-N
Formula: C13H24O2
SMILES: C=CCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
af	0.6737		Cheméo Relay (1.0)
gf	-87.50	kJ/mol	Joback Method
hf	-507.72	kJ/mol	Cheméo Relay (1.0)
hfus	30.93	kJ/mol	Joback Method
hvap	76.92	kJ/mol	Cheméo Relay (1.0)
ie	9.45	eV	Cheméo Relay (1.0)
log10ws	-4.35		Cheméo Relay (1.0)
logp	3.856		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
ripol	2397.00		NIST Webbook
ripol	2397.00		NIST Webbook
ripol	2397.00		NIST Webbook
tb	528.89	K	Cheméo Relay (1.0)
tc	709.89	K	Cheméo Relay (1.0)
tf	264.17	K	Cheméo Relay (1.0)
vc	0.737	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.21	J/mol×K	569.81	Joback Method
cpg	510.03	J/mol×K	598.38	Joback Method
cpg	525.18	J/mol×K	626.96	Joback Method
cpg	539.69	J/mol×K	655.53	Joback Method

cpg	553.58	J/mol×K	684.10	Joback Method
cpg	566.84	J/mol×K	712.68	Joback Method
cpg	579.50	J/mol×K	741.25	Joback Method
dvisc	0.0027987	Pa×s	306.67	Joback Method
dvisc	0.0013224	Pa×s	350.53	Joback Method
dvisc	0.0007382	Pa×s	394.38	Joback Method
dvisc	0.0004631	Pa×s	438.24	Joback Method
dvisc	0.0003162	Pa×s	482.10	Joback Method
dvisc	0.0002301	Pa×s	525.95	Joback Method
dvisc	0.0001759	Pa×s	569.81	Joback Method

Sources

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=C29972790&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume