methyl 3-decenoate

Inchi: InChI=1S/C11H20O2/c1-3-4-5-6-7-8-9-10-11(12)13-2/h8-9H,3-7,10H2,1-2H3/b9-8+
InchiKey: HLXICRJOFXSTBV-CMDGGOBGSA-N
Formula: C11H20O2
SMILES: CCCCCC/C=C/CC(=O)OC
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
af	0.5324		Cheméo Relay (1.0)
gf	-188.41	kJ/mol	Joback Method
hf	-468.88	kJ/mol	Cheméo Relay (1.0)
hfus	28.82	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-3.83		Cheméo Relay (1.0)
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1321.00		NIST Webbook
rinpol	1321.00		NIST Webbook
tb	485.04	K	Cheméo Relay (1.0)
tc	681.44	K	Cheméo Relay (1.0)
tf	222.12	K	Cheméo Relay (1.0)
vc	0.619	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	4.11600e+00
Coeff. B	1.01404e+00
Coeff. C	-5.63800e-04

Coeff. D	1.10000e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.20675e+01
Coeff. B	1.71216e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	250.98
Temperature range (K), max.	482.30

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R218227&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):

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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