ethyl (Z)-6-nonenoate

Inchi: InChI=1S/C11H20O2/c1-3-5-6-7-8-9-10-11(12)13-4-2/h5-6H,3-4,7-10H2,1-2H3/b6-5-
InchiKey: CGLQUAOCIKSACB-WAYWQWQTSA-N
Formula: C11H20O2
SMILES: CCC=CCCCCC(=O)OCC
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-111.96	kJ/mol	Joback Method
hf	-397.95	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
ripol	1609.00		NIST Webbook
ripol	1609.00		NIST Webbook
tb	531.53	K	Joback Method
tc	709.61	K	Joback Method
tf	280.81	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.35	J/mol×K	531.53	Joback Method
cpg	411.96	J/mol×K	561.21	Joback Method
cpg	425.95	J/mol×K	590.89	Joback Method
cpg	439.33	J/mol×K	620.57	Joback Method
cpg	452.12	J/mol×K	650.25	Joback Method
cpg	464.33	J/mol×K	679.93	Joback Method
cpg	475.98	J/mol×K	709.61	Joback Method
dvisc	0.0029775	Pa×s	280.81	Joback Method

dvisc	0.0013650	Pa×s	322.60	Joback Method
dvisc	0.0007484	Pa×s	364.38	Joback Method
dvisc	0.0004643	Pa×s	406.17	Joback Method
dvisc	0.0003149	Pa×s	447.96	Joback Method
dvisc	0.0002282	Pa×s	489.74	Joback Method
dvisc	0.0001740	Pa×s	531.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
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

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