propyl 7-octenoate

Inchi: InChI=1S/C11H20O2/c1-3-5-6-7-8-9-11(12)13-10-4-2/h3H,1,4-10H2,2H3
InchiKey: KJBRZWADVLEUIE-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: C=CCCCCCC(=O)OCCC
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-104.34	kJ/mol	Joback Method
hf	-389.74	kJ/mol	Joback Method
hfus	25.75	kJ/mol	Joback Method
hvap	48.57	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
ripol	1556.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1556.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1556.00		NIST Webbook
tb	524.05	K	Joback Method
tc	698.08	K	Joback Method
tf	284.13	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.19	J/mol×K	524.05	Joback Method
cpg	410.62	J/mol×K	553.05	Joback Method
cpg	424.47	J/mol×K	582.06	Joback Method
cpg	437.74	J/mol×K	611.06	Joback Method
cpg	450.46	J/mol×K	640.07	Joback Method

cpg	462.62	J/mol×K	669.07	Joback Method
cpg	474.25	J/mol×K	698.08	Joback Method
dvisc	0.0029982	Pa×s	284.13	Joback Method
dvisc	0.0014650	Pa×s	324.12	Joback Method
dvisc	0.0008378	Pa×s	364.10	Joback Method
dvisc	0.0005351	Pa×s	404.09	Joback Method
dvisc	0.0003706	Pa×s	444.08	Joback Method
dvisc	0.0002727	Pa×s	484.06	Joback Method
dvisc	0.0002102	Pa×s	524.05	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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