propyl octanoate-d15

Inchi: InChI=1S/C11H22O2/c1-3-5-6-7-8-9-11(12)13-10-4-2/h3-10H2,1-2H3/i1D3,3D2,5D2,6D2
InchiKey: IDHBLVYDNJDWNO-MVIIYOROSA-N
Formula: C11H7D15O2
SMILES: CCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 201.38

Physical Properties

Property code	Value	Unit	Source
gf	-192.18	kJ/mol	Joback Method
hf	-515.17	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.300		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
ripol	1506.00		NIST Webbook
ripol	1506.00		NIST Webbook
tb	527.37	K	Joback Method
tc	698.36	K	Joback Method
tf	285.89	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.24	J/mol×K	527.37	Joback Method
cpg	430.19	J/mol×K	555.87	Joback Method
cpg	444.58	J/mol×K	584.37	Joback Method
cpg	458.41	J/mol×K	612.87	Joback Method
cpg	471.67	J/mol×K	641.36	Joback Method
cpg	484.39	J/mol×K	669.86	Joback Method
cpg	496.57	J/mol×K	698.36	Joback Method
dvisc	0.0032030	Pa×s	285.89	Joback Method

dvisc	0.0015281	Pa×s	326.14	Joback Method
dvisc	0.0008577	Pa×s	366.38	Joback Method
dvisc	0.0005398	Pa×s	406.63	Joback Method
dvisc	0.0003692	Pa×s	446.88	Joback Method
dvisc	0.0002689	Pa×s	487.12	Joback Method
dvisc	0.0002056	Pa×s	527.37	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=R329189&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