propyl hexanoate-d3

Inchi: InChI=1S/C9H18O2/c1-3-5-6-7-9(10)11-8-4-2/h3-8H2,1-2H3/i1D3
InchiKey: HTUIWRWYYVBCFT-FIBGUPNXSA-N
Formula: C9H15D3O2
SMILES: CCCCCC(=O)OCCC
Mol. weight [g/mol]: 161.26

Physical Properties

Property code	Value	Unit	Source
gf	-209.02	kJ/mol	Joback Method
hf	-473.89	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	44.78	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.520		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
ripol	1312.00		NIST Webbook
tb	481.61	K	Joback Method
tc	655.29	K	Joback Method
tf	263.35	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.89	J/mol×K	481.61	Joback Method
cpg	336.15	J/mol×K	510.56	Joback Method
cpg	348.92	J/mol×K	539.50	Joback Method
cpg	361.21	J/mol×K	568.45	Joback Method
cpg	373.04	J/mol×K	597.40	Joback Method
cpg	384.40	J/mol×K	626.35	Joback Method
cpg	395.29	J/mol×K	655.29	Joback Method
dvisc	0.0033103	Pa×s	263.35	Joback Method
dvisc	0.0016384	Pa×s	299.73	Joback Method

dvisc	0.0009442	Pa×s	336.10	Joback Method
dvisc	0.0006060	Pa×s	372.48	Joback Method
dvisc	0.0004209	Pa×s	408.86	Joback Method
dvisc	0.0003103	Pa×s	445.23	Joback Method
dvisc	0.0002395	Pa×s	481.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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