ethyl hexanoate-d11

Inchi: InChI=1S/C8H16O2/c1-3-5-6-7-8(9)10-4-2/h3-7H2,1-2H3/i1D3,3D2,5D2,6D2,7D2
InchiKey: SHZIWNPUGXLXDT-LELBNVJRSA-N
Formula: C8H5D11O2
SMILES: CCCCCC(=O)OCC
Mol. weight [g/mol]: 155.28

Physical Properties

Property code	Value	Unit	Source
gf	-217.44	kJ/mol	Joback Method
hf	-453.25	kJ/mol	Joback Method
hfus	19.26	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.130		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
ripol	1226.00		NIST Webbook
ripol	1226.00		NIST Webbook
tb	458.73	K	Joback Method
tc	633.80	K	Joback Method
tf	252.08	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.70	J/mol×K	458.73	Joback Method
cpg	291.94	J/mol×K	487.91	Joback Method
cpg	303.75	J/mol×K	517.09	Joback Method
cpg	315.14	J/mol×K	546.26	Joback Method
cpg	326.10	J/mol×K	575.44	Joback Method
cpg	336.64	J/mol×K	604.62	Joback Method
cpg	346.77	J/mol×K	633.80	Joback Method
dvisc	0.0032831	Pa×s	252.08	Joback Method

dvisc	0.0016585	Pa×s	286.52	Joback Method
dvisc	0.0009701	Pa×s	320.96	Joback Method
dvisc	0.0006296	Pa×s	355.40	Joback Method
dvisc	0.0004410	Pa×s	389.85	Joback Method
dvisc	0.0003273	Pa×s	424.29	Joback Method
dvisc	0.0002540	Pa×s	458.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R328993&Units=SI

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