hexyl-d11 acetate

Inchi: InChI=1S/C6H14O/c1-2-3-4-5-6-7/h7H,2-6H2,1H3/i1D3,2D2,3D2,4D2,5D2
InchiKey: ZSIAUFGUXNUGDI-GILSBCIXSA-N
Formula: C6H3D11O
SMILES: CCCCCCO
Mol. weight [g/mol]: 113.24

Physical Properties

Property code	Value	Unit	Source
gf	-137.18	kJ/mol	Joback Method
hf	-319.40	kJ/mol	Joback Method
hfus	15.38	kJ/mol	Joback Method
hvap	45.63	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.559		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
ripol	1266.00		NIST Webbook
ripol	1266.00		NIST Webbook
tb	428.86	K	Joback Method
tc	589.96	K	Joback Method
tf	218.20	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.67	J/mol×K	428.86	Joback Method
cpg	217.18	J/mol×K	455.71	Joback Method
cpg	226.36	J/mol×K	482.56	Joback Method
cpg	235.20	J/mol×K	509.41	Joback Method
cpg	243.71	J/mol×K	536.26	Joback Method
cpg	251.90	J/mol×K	563.11	Joback Method
cpg	259.79	J/mol×K	589.96	Joback Method
dvisc	0.0859852	Pa×s	218.20	Joback Method

dvisc	0.0165401	Pa×s	253.31	Joback Method
dvisc	0.0047527	Pa×s	288.42	Joback Method
dvisc	0.0017902	Pa×s	323.53	Joback Method
dvisc	0.0008164	Pa×s	358.64	Joback Method
dvisc	0.0004282	Pa×s	393.75	Joback Method
dvisc	0.0002497	Pa×s	428.86	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=R329030&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