

3E-hexenyl-d3 acetate

Inchi:	InChI=1S/C8H14O2/c1-3-4-5-6-7-10-8(2)9/h4-5H,3,6-7H2,1-2H3/b5-4+/i1D3
InchiKey:	NPFVVOOAXDOBMCE-TYYDCBDZSA-N
Formula:	C8H11D3O2
SMILES:	CCC=CCCOC(C)=O
Mol. weight [g/mol]:	145.21

Physical Properties

Property code	Value	Unit	Source
gf	-137.22	kJ/mol	Joback Method
hf	-336.03	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	42.52	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.906		Crippen Method
mvol	126.720	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
ripol	1301.00		NIST Webbook
ripol	1301.00		NIST Webbook
tb	462.89	K	Joback Method
tc	646.21	K	Joback Method
tf	247.00	K	Joback Method
vc	0.487	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.30	J/molxK	462.89	Joback Method
cpg	275.19	J/molxK	493.44	Joback Method
cpg	286.60	J/molxK	524.00	Joback Method
cpg	297.52	J/molxK	554.55	Joback Method
cpg	307.96	J/molxK	585.10	Joback Method
cpg	317.95	J/molxK	615.66	Joback Method
cpg	327.49	J/molxK	646.21	Joback Method
dvisc	0.0030324	Paxs	247.00	Joback Method

dvisc	0.0014687	Paxs	282.98	Joback Method
dvisc	0.0008378	Paxs	318.96	Joback Method
dvisc	0.0005355	Paxs	354.94	Joback Method
dvisc	0.0003717	Paxs	390.93	Joback Method
dvisc	0.0002744	Paxs	426.91	Joback Method
dvisc	0.0002123	Paxs	462.89	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=R328740&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

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