

hexyl-d3 acetate

Inchi:	InChI=1S/C8H16O2/c1-3-4-5-6-7-10-8(2)9/h3-7H2,1-2H3/i1D3
InchiKey:	AOGQPLXWSUTHQB-FIBGUPNXSA-N
Formula:	C8H13D3O2
SMILES:	CCCCCOC(C)=O
Mol. weight [g/mol]:	147.23

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	1270.00		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/molxK	458.73	Joback Method
cpg	291.94	J/molxK	487.91	Joback Method
cpg	303.75	J/molxK	517.09	Joback Method
cpg	315.14	J/molxK	546.26	Joback Method
cpg	326.10	J/molxK	575.44	Joback Method
cpg	336.64	J/molxK	604.62	Joback Method
cpg	346.77	J/molxK	633.80	Joback Method
dvisc	0.0032831	Paxs	252.08	Joback Method
dvisc	0.0016585	Paxs	286.52	Joback Method

dvisc	0.0009701	Paxs	320.96	Joback Method
dvisc	0.0006296	Paxs	355.40	Joback Method
dvisc	0.0004410	Paxs	389.85	Joback Method
dvisc	0.0003273	Paxs	424.29	Joback Method
dvisc	0.0002540	Paxs	458.73	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=R329050&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
mccvol:	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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