

2E-hexenyl-d3 proprionate

Inchi:	InChI=1S/C9H16O2/c1-3-5-6-7-8-11-9(10)4-2/h6-7H,3-5,8H2,1-2H3/b7-6+/i1D3
InchiKey:	LPWKTEHEFDVAQS-ZRNNCLBUSA-N
Formula:	C9H13D3O2
SMILES:	CCCC=CCOC(=O)CC
Mol. weight [g/mol]:	159.24

Physical Properties

Property code	Value	Unit	Source
gf	-128.80	kJ/mol	Joback Method
hf	-356.67	kJ/mol	Joback Method
hfus	22.05	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mvol	140.810	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
ripol	1393.00		NIST Webbook
ripol	1393.00		NIST Webbook
tb	485.77	K	Joback Method
tc	667.32	K	Joback Method
tf	258.27	K	Joback Method
vc	0.543	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.02	J/molxK	485.77	Joback Method
cpg	318.93	J/molxK	516.03	Joback Method
cpg	331.30	J/molxK	546.29	Joback Method
cpg	343.15	J/molxK	576.54	Joback Method
cpg	354.47	J/molxK	606.80	Joback Method
cpg	365.29	J/molxK	637.06	Joback Method
cpg	375.62	J/molxK	667.32	Joback Method
dvisc	0.0030655	Paxs	258.27	Joback Method

dvisc	0.0014558	Paxs	296.19	Joback Method
dvisc	0.0008186	Paxs	334.10	Joback Method
dvisc	0.0005177	Paxs	372.02	Joback Method
dvisc	0.0003563	Paxs	409.94	Joback Method
dvisc	0.0002612	Paxs	447.85	Joback Method
dvisc	0.0002011	Paxs	485.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R328715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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