

3E-hexenyl-d3 hexanoate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H22O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h5,7H,3-4,6,8-11H2,1-2H3/b7-5

RGACQXBDYBCJCY-PKJLGKQPSA-N

C12H19D3O2

CCC=CCCOC(=O)CCCCC

201.32

Physical Properties

Property code	Value	Unit	Source
gf	-103.54	kJ/mol	Joback Method
hf	-418.59	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
ripol	1646.00		NIST Webbook
ripol	1646.00		NIST Webbook
tb	554.41	K	Joback Method
tc	730.90	K	Joback Method
tf	292.08	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.74	J/molxK	554.41	Joback Method
cpg	515.92	J/molxK	701.48	Joback Method
cpg	503.13	J/molxK	672.07	Joback Method
cpg	489.74	J/molxK	642.65	Joback Method
cpg	475.72	J/molxK	613.24	Joback Method
cpg	461.06	J/molxK	583.82	Joback Method
cpg	528.11	J/molxK	730.90	Joback Method
dvisc	0.0001595	Paxs	554.41	Joback Method

dvisc	0.0002101	Paxs	510.69	Joback Method
dvisc	0.0002914	Paxs	466.97	Joback Method
dvisc	0.0004324	Paxs	423.25	Joback Method
dvisc	0.0007029	Paxs	379.52	Joback Method
dvisc	0.0012967	Paxs	335.80	Joback Method
dvisc	0.0028734	Paxs	292.08	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=R328775&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

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