

3E-hexenyl-d3 butanoate-d3

Inchi:	InChI=1S/C10H18O2/c1-3-5-6-7-9-12-10(11)8-4-2/h5-6H,3-4,7-9H2,1-2H3/b6-5+/i1D3,2D
InchiKey:	ZCHOPXVYTWUHDS-MPLSCHIPSA-N
Formula:	C10H12D6O2
SMILES:	CCC=CCCOC(=O)CCC
Mol. weight [g/mol]:	176.29

Physical Properties

Property code	Value	Unit	Source
gf	-120.38	kJ/mol	Joback Method
hf	-377.31	kJ/mol	Joback Method
hfus	24.64	kJ/mol	Joback Method
hvap	46.97	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.686		Crippen Method
mvol	154.900	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
ripol	1447.00		NIST Webbook
ripol	1447.00		NIST Webbook
tb	508.65	K	Joback Method
tc	688.43	K	Joback Method
tf	269.54	K	Joback Method
vc	0.600	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.74	J/molxK	508.65	Joback Method
cpg	364.56	J/molxK	538.61	Joback Method
cpg	377.79	J/molxK	568.58	Joback Method
cpg	390.44	J/molxK	598.54	Joback Method
cpg	402.54	J/molxK	628.50	Joback Method
cpg	414.10	J/molxK	658.47	Joback Method
cpg	425.13	J/molxK	688.43	Joback Method
dvisc	0.0030444	Paxs	269.54	Joback Method

dvisc	0.0014196	Paxs	309.39	Joback Method
dvisc	0.0007878	Paxs	349.24	Joback Method
dvisc	0.0004933	Paxs	389.10	Joback Method
dvisc	0.0003369	Paxs	428.95	Joback Method
dvisc	0.0002455	Paxs	468.80	Joback Method
dvisc	0.0001880	Paxs	508.65	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R328760&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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