3E-hexenyl-d3 butanoate

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
InchiKey: ZCHOPXVYTWUHDS-KWUDEMAWSA-N
Formula: C10H15D3O2
SMILES: CCC=CCCOC(=O)CCC
Mol. weight [g/mol]: 173.27

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
mcvol	154.900	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
ripol	1450.00		NIST Webbook
ripol	1450.00		NIST Webbook
tb	508.65	K	Joback Method
tc	688.43	K	Joback Method
tf	269.54	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0014196	Pa×s	309.39	Joback Method
dvisc	0.0007878	Pa×s	349.24	Joback Method
dvisc	0.0004933	Pa×s	389.10	Joback Method
dvisc	0.0003369	Pa×s	428.95	Joback Method
dvisc	0.0002455	Pa×s	468.80	Joback Method
dvisc	0.0001880	Pa×s	508.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R328755&Units=SI
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

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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