

butyl-d3 hexanoate-d3

Inchi:	InChI=1S/C10H20O2/c1-3-5-7-8-10(11)12-9-6-4-2/h3-9H2,1-2H3/i1D3,2D3
InchiKey:	RPRPDTXKGSIXMD-WFGJKAKNSA-N
Formula:	C10H14D6O2
SMILES:	CCCCC(=O)OCCCC
Mol. weight [g/mol]:	178.30

Physical Properties

Property code	Value	Unit	Source
gf	-200.60	kJ/mol	Joback Method
hf	-494.53	kJ/mol	Joback Method
hfus	24.44	kJ/mol	Joback Method
hvap	47.01	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.910		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
ripol	1402.00		NIST Webbook
tb	504.49	K	Joback Method
tc	676.79	K	Joback Method
tf	274.62	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.11	J/molxK	504.49	Joback Method
cpg	382.26	J/molxK	533.21	Joback Method
cpg	395.89	J/molxK	561.92	Joback Method
cpg	409.00	J/molxK	590.64	Joback Method
cpg	421.59	J/molxK	619.36	Joback Method
cpg	433.67	J/molxK	648.08	Joback Method
cpg	445.25	J/molxK	676.79	Joback Method
dvisc	0.0032806	Paxs	274.62	Joback Method
dvisc	0.0015931	Paxs	312.93	Joback Method

dvisc	0.0009057	Paxs	351.24	Joback Method
dvisc	0.0005753	Paxs	389.56	Joback Method
dvisc	0.0003964	Paxs	427.87	Joback Method
dvisc	0.0002904	Paxs	466.18	Joback Method
dvisc	0.0002230	Paxs	504.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R328913&Units=SI
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

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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