

2-methylbutyl-d-9 acetate

Inchi:	InChI=1S/C7H14O2/c1-4-6(2)5-9-7(3)8/h6H,4-5H2,1-3H3/i1D3,2D3,4D2,6D
InchiKey:	XHIUFYZDQBSEMF-YMNJYQJHSA-N
Formula:	C7H5D9O2
SMILES:	CCC(C)COC(C)=O
Mol. weight [g/mol]:	139.24

Physical Properties

Property code	Value	Unit	Source
gf	-228.30	kJ/mol	Joback Method
hf	-437.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	39.94	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
ripol	1126.00		NIST Webbook
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tb	435.41	K	Joback Method
tc	615.76	K	Joback Method
tf	225.81	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.73	J/molxK	435.41	Joback Method
cpg	291.98	J/molxK	585.70	Joback Method
cpg	282.12	J/molxK	555.64	Joback Method
cpg	271.87	J/molxK	525.58	Joback Method
cpg	261.22	J/molxK	495.53	Joback Method
cpg	250.17	J/molxK	465.47	Joback Method
cpg	301.45	J/molxK	615.76	Joback Method
dvisc	0.0002542	Paxs	435.41	Joback Method

dvisc	0.0003348	Paxs	400.48	Joback Method
dvisc	0.0004649	Paxs	365.54	Joback Method
dvisc	0.0006919	Paxs	330.61	Joback Method
dvisc	0.0011312	Paxs	295.68	Joback Method
dvisc	0.0021099	Paxs	260.74	Joback Method
dvisc	0.0047724	Paxs	225.81	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=R322628&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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