

butyl-d3 acetate

Inchi:	InChI=1S/C6H12O2/c1-3-4-5-8-6(2)7/h3-5H2,1-2H3/i1D3
InchiKey:	DKPFZGUDAPQIHT-FIBGUPNXSA-N
Formula:	C6H9D3O2
SMILES:	CCCCOC(C)=O
Mol. weight [g/mol]:	119.18

Physical Properties

Property code	Value	Unit	Source
gf	-234.28	kJ/mol	Joback Method
hf	-411.97	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	38.11	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.350		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
ripol	1073.00		NIST Webbook
ripol	1073.00		NIST Webbook
tb	412.97	K	Joback Method
tc	590.55	K	Joback Method
tf	229.54	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.87	J/molxK	412.97	Joback Method
cpg	209.71	J/molxK	442.57	Joback Method
cpg	219.25	J/molxK	472.16	Joback Method
cpg	228.47	J/molxK	501.76	Joback Method
cpg	237.38	J/molxK	531.36	Joback Method
cpg	245.98	J/molxK	560.96	Joback Method
cpg	254.27	J/molxK	590.55	Joback Method
dvisc	0.0030279	Paxs	229.54	Joback Method

dvisc	0.0016017	Paxs	260.11	Joback Method
dvisc	0.0009687	Paxs	290.68	Joback Method
dvisc	0.0006447	Paxs	321.25	Joback Method
dvisc	0.0004605	Paxs	351.83	Joback Method
dvisc	0.0003472	Paxs	382.40	Joback Method
dvisc	0.0002729	Paxs	412.97	Joback Method

Sources

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=R328884&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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