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/mol×K	412.97	Joback Method
cpg	209.71	J/mol×K	442.57	Joback Method
cpg	219.25	J/mol×K	472.16	Joback Method
cpg	228.47	J/mol×K	501.76	Joback Method
cpg	237.38	J/mol×K	531.36	Joback Method
cpg	245.98	J/mol×K	560.96	Joback Method
cpg	254.27	J/mol×K	590.55	Joback Method
dvisc	0.0030279	Pa×s	229.54	Joback Method

dvisc	0.0016017	Pa×s	260.11	Joback Method
dvisc	0.0009687	Pa×s	290.68	Joback Method
dvisc	0.0006447	Pa×s	321.25	Joback Method
dvisc	0.0004605	Pa×s	351.83	Joback Method
dvisc	0.0003472	Pa×s	382.40	Joback Method
dvisc	0.0002729	Pa×s	412.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R328884&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
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