butyl 2-methylbutanoate-d-3

Inchi: InChI=1S/C9H18O2/c1-4-6-7-11-9(10)8(3)5-2/h8H,4-7H2,1-3H3/i2D3
InchiKey: OTKQNSSMCDLVQV-BMSJAHLVSA-N
Formula: C9H15D3O2
SMILES: CCCCOC(=O)C(C)CC
Mol. weight [g/mol]: 161.26

Physical Properties

Property code	Value	Unit	Source
gf	-211.46	kJ/mol	Joback Method
hf	-479.17	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	44.40	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.376		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
ripol	1237.00		NIST Webbook
ripol	1237.00		NIST Webbook
tb	481.17	K	Joback Method
tc	658.49	K	Joback Method
tf	248.35	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.06	J/mol×K	481.17	Joback Method
cpg	336.66	J/mol×K	510.72	Joback Method
cpg	349.76	J/mol×K	540.28	Joback Method
cpg	362.35	J/mol×K	569.83	Joback Method
cpg	374.44	J/mol×K	599.38	Joback Method
cpg	386.04	J/mol×K	628.93	Joback Method
cpg	397.15	J/mol×K	658.49	Joback Method
dvisc	0.0047844	Pa×s	248.35	Joback Method

dvisc	0.0020429	Pa×s	287.15	Joback Method
dvisc	0.0010682	Pa×s	325.96	Joback Method
dvisc	0.0006412	Pa×s	364.76	Joback Method
dvisc	0.0004246	Pa×s	403.56	Joback Method
dvisc	0.0003022	Pa×s	442.37	Joback Method
dvisc	0.0002272	Pa×s	481.17	Joback Method

Sources

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=R322653&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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