

methyl 2-methylbutanoate-d-9

Inchi:	InChI=1S/C6H12O2/c1-4-5(2)6(7)8-3/h5H,4H2,1-3H3/i1D3,2D3,4D2,5D
InchiKey:	OCWLYWIFNDCWRZ-OMLAQRBSSA-N
Formula:	C6H3D9O2
SMILES:	CCC(C)C(=O)OC
Mol. weight [g/mol]:	125.21

Physical Properties

Property code	Value	Unit	Source
gf	-236.72	kJ/mol	Joback Method
hf	-417.25	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	37.72	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	1.205		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
ripol	1003.00		NIST Webbook
tb	412.53	K	Joback Method
tc	594.22	K	Joback Method
tf	214.54	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.90	J/molxK	412.53	Joback Method
cpg	210.06	J/molxK	442.81	Joback Method
cpg	219.89	J/molxK	473.09	Joback Method
cpg	229.39	J/molxK	503.38	Joback Method
cpg	238.55	J/molxK	533.66	Joback Method
cpg	247.38	J/molxK	563.94	Joback Method
cpg	255.87	J/molxK	594.22	Joback Method
dvisc	0.0046134	Paxs	214.54	Joback Method
dvisc	0.0020807	Paxs	247.54	Joback Method

dvisc	0.0011317	Paxs	280.54	Joback Method
dvisc	0.0006998	Paxs	313.53	Joback Method
dvisc	0.0004742	Paxs	346.53	Joback Method
dvisc	0.0003438	Paxs	379.53	Joback Method
dvisc	0.0002624	Paxs	412.53	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=R322722&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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