2-Pentanone, 4-methyl-1,1,1,3,3-d5-

Inchi: InChI=1S/C6H12O/c1-5(2)4-6(3)7/h5H,4H2,1-3H3/i3D3,4D2
InchiKey: NTIZESTWPVYFNL-IKISXXDZSA-N
Formula: C6H7D5O
SMILES: CC(=O)CC(C)C
Mol. weight [g/mol]: 105.19
CAS: 4840-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-131.72	kJ/mol	Joback Method
hf	-285.03	kJ/mol	Joback Method
hfus	9.37	kJ/mol	Joback Method
hvap	35.31	kJ/mol	Joback Method
ie	9.35	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.621		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	390.11	K	Joback Method
tc	571.85	K	Joback Method
tf	192.31	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.67	J/mol×K	390.11	Joback Method
cpg	188.09	J/mol×K	420.40	Joback Method
cpg	198.11	J/mol×K	450.69	Joback Method
cpg	207.72	J/mol×K	480.98	Joback Method
cpg	216.93	J/mol×K	511.27	Joback Method
cpg	225.77	J/mol×K	541.56	Joback Method
cpg	234.22	J/mol×K	571.85	Joback Method
dvisc	0.0061867	Pa×s	192.31	Joback Method

dvisc	0.0025603	Pa×s	225.28	Joback Method
dvisc	0.0013273	Pa×s	258.24	Joback Method
dvisc	0.0007984	Pa×s	291.21	Joback Method
dvisc	0.0005326	Pa×s	324.18	Joback Method
dvisc	0.0003828	Pa×s	357.14	Joback Method
dvisc	0.0002910	Pa×s	390.11	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4840817&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume