Acetophenone-«alpha»,«alpha»,«alpha»-d3

Inchi: InChI=1S/C8H8O/c1-7(9)8-5-3-2-4-6-8/h2-6H,1H3/i1D3
InchiKey: KWOLFJPFCHCOCG-FIBGUPNXSA-N
Formula: C8H5D3O
SMILES: CC(=O)c1ccccc1
Mol. weight [g/mol]: 123.17
CAS: 17537-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-0.03	kJ/mol	Joback Method
hf	-84.50	kJ/mol	Joback Method
hfus	12.12	kJ/mol	Joback Method
hvap	42.42	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.889		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
tb	462.99	K	Joback Method
tc	684.79	K	Joback Method
tf	256.27	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.32	J/mol×K	462.99	Joback Method
cpg	204.10	J/mol×K	499.96	Joback Method
cpg	215.13	J/mol×K	536.92	Joback Method
cpg	225.45	J/mol×K	573.89	Joback Method
cpg	235.08	J/mol×K	610.86	Joback Method
cpg	244.05	J/mol×K	647.82	Joback Method
cpg	252.40	J/mol×K	684.79	Joback Method
dvisc	0.0029135	Pa×s	256.27	Joback Method
dvisc	0.0015654	Pa×s	290.72	Joback Method

dvisc	0.0009594	Pa×s	325.18	Joback Method
dvisc	0.0006459	Pa×s	359.63	Joback Method
dvisc	0.0004659	Pa×s	394.08	Joback Method
dvisc	0.0003542	Pa×s	428.54	Joback Method
dvisc	0.0002805	Pa×s	462.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17537314&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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