[1,1,1-2H3]-4-Benzyloxy-2-butanone

Inchi: InChI=1S/C11H14O2/c1-10(12)7-8-13-9-11-5-3-2-4-6-11/h2-6H,7-9H2,1H3/i1D3
InchiKey: BTOZGSIVAZGXCH-FIBGUPNXSA-N
Formula: C11H11D3O2
SMILES: CC(=O)CCOCc1ccccc1
Mol. weight [g/mol]: 181.25

Physical Properties

Property code	Value	Unit	Source
gf	-79.77	kJ/mol	Joback Method
hf	-278.64	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.182		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1463.00		NIST Webbook
rinpol	1463.00		NIST Webbook
tb	554.05	K	Joback Method
tc	763.32	K	Joback Method
tf	312.31	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.39	J/mol×K	554.05	Joback Method
cpg	360.84	J/mol×K	588.93	Joback Method
cpg	374.48	J/mol×K	623.81	Joback Method
cpg	387.33	J/mol×K	658.68	Joback Method
cpg	399.42	J/mol×K	693.56	Joback Method
cpg	410.76	J/mol×K	728.44	Joback Method
cpg	421.37	J/mol×K	763.32	Joback Method
dvisc	0.0023060	Pa×s	312.31	Joback Method

dvisc	0.0012165	Pa×s	352.60	Joback Method
dvisc	0.0007317	Pa×s	392.89	Joback Method
dvisc	0.0004838	Pa×s	433.18	Joback Method
dvisc	0.0003432	Pa×s	473.47	Joback Method
dvisc	0.0002569	Pa×s	513.76	Joback Method
dvisc	0.0002006	Pa×s	554.05	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=R412390&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume