

[1,1,1,3,3-2H5]-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/i1D3,7D2
InchiKey:	BTOZGSIVA ZGXCH-WRMAMSRYSA-N
Formula:	C11H9D5O2
SMILES:	CC(=O)CCOCc1ccccc1
Mol. weight [g/mol]:	183.26

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
rinsol	1458.00		NIST Webbook
tb	554.05	K	Joback Method
tc	763.32	K	Joback Method
tf	312.31	K	Joback Method
vc	0.568	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.39	J/molxK	554.05	Joback Method
cpg	360.84	J/molxK	588.93	Joback Method
cpg	374.48	J/molxK	623.81	Joback Method
cpg	387.33	J/molxK	658.68	Joback Method
cpg	399.42	J/molxK	693.56	Joback Method
cpg	410.76	J/molxK	728.44	Joback Method
cpg	421.37	J/molxK	763.32	Joback Method
dvisc	0.0023060	Paxs	312.31	Joback Method
dvisc	0.0012165	Paxs	352.60	Joback Method

dvisc	0.0007317	Paxs	392.89	Joback Method
dvisc	0.0004838	Paxs	433.18	Joback Method
dvisc	0.0003432	Paxs	473.47	Joback Method
dvisc	0.0002569	Paxs	513.76	Joback Method
dvisc	0.0002006	Paxs	554.05	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=R412409&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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