

BUTANAL, 4-[(TETRAHYDRO-2H-PYRAN-2-YL)OXY]-

Other names:	4-(2-Tetrahydropyranyloxy)butanal
Inchi:	InChI=1S/C9H16O3/c10-6-2-4-8-12-9-5-1-3-7-11-9/h6,9H,1-5,7-8H2
InchiKey:	UWMPHMYUITTYTD-UHFFFAOYSA-N
Formula:	C9H16O3
SMILES:	O=CCCCOC1CCCCO1
Mol. weight [g/mol]:	172.22

Physical Properties

Property code	Value	Unit	Source
hfus	22.36	kJ/mol	Joback Method
hvap	59.78	kJ/mol	Cheméo Relay (1.0)
logp	1.509		Crippen Method
mcvol	140.120	ml/mol	McGowan Method
rinpol	1322.00		NIST Webbook
rinpol	1322.00		NIST Webbook
tb	513.68	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.55	J/mol×K	522.90	Joback Method
cpg	425.11	J/mol×K	724.98	Joback Method
cpg	412.93	J/mol×K	691.30	Joback Method
cpg	400.00	J/mol×K	657.62	Joback Method
cpg	386.30	J/mol×K	623.94	Joback Method
cpg	371.83	J/mol×K	590.26	Joback Method
cpg	356.58	J/mol×K	556.58	Joback Method
dvisc	0.0007827	Pa×s	406.13	Joback Method
dvisc	0.0002872	Pa×s	522.90	Joback Method
dvisc	0.0003801	Pa×s	483.98	Joback Method
dvisc	0.0005285	Pa×s	445.06	Joback Method
dvisc	0.0047923	Pa×s	289.37	Joback Method
dvisc	0.0012598	Pa×s	367.21	Joback Method
dvisc	0.0022700	Pa×s	328.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54911852&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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