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
CAS: 54911-85-2

Physical Properties

Property code	Value	Unit	Source
gf	-241.29	kJ/mol	Joback Method
hf	-524.57	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.509		Crippen Method
mcvol	140.120	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1322.00		NIST Webbook
rinpol	1322.00		NIST Webbook
tb	522.90	K	Joback Method
tc	724.98	K	Joback Method
tf	289.37	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.55	J/mol×K	522.90	Joback Method
cpg	356.58	J/mol×K	556.58	Joback Method
cpg	371.83	J/mol×K	590.26	Joback Method
cpg	386.30	J/mol×K	623.94	Joback Method
cpg	400.00	J/mol×K	657.62	Joback Method
cpg	412.93	J/mol×K	691.30	Joback Method

cpg	425.11	J/mol×K	724.98	Joback Method
dvisc	0.0047923	Pa×s	289.37	Joback Method
dvisc	0.0022700	Pa×s	328.29	Joback Method
dvisc	0.0012598	Pa×s	367.21	Joback Method
dvisc	0.0007827	Pa×s	406.13	Joback Method
dvisc	0.0005285	Pa×s	445.06	Joback Method
dvisc	0.0003801	Pa×s	483.98	Joback Method
dvisc	0.0002872	Pa×s	522.90	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54911852&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.