

2-Octenal, 2-butyl-

Other names:	2-Butyl-2-octenal 2-n-Butyloct-2-enal 2-Octenal, 2-butyl, (Z)-
Inchi:	InChI=1S/C12H22O/c1-3-5-7-8-10-12(11-13)9-6-4-2/h10-11H,3-9H2,1-2H3/b12-10-
InchiKey:	LYGMPIZYNJGJKP-BENRWUELSA-N
Formula:	C12H22O
SMILES:	CCCCC=C(C=O)CCCC
Mol. weight [g/mol]:	182.30
CAS:	13019-16-4

Physical Properties

Property code	Value	Unit	Source
gf	22.31	kJ/mol	Joback Method
hf	-269.16	kJ/mol	Joback Method
hfus	28.02	kJ/mol	Joback Method
hvap	49.06	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.882		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
ripol	1372.20		NIST Webbook
ripol	1367.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1389.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1363.00		NIST Webbook
ripol	1389.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1359.00		NIST Webbook
ripol	1372.20		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1659.00		NIST Webbook
ripol	1653.00		NIST Webbook

ripol	1659.00		NIST Webbook
tb	526.66	K	Joback Method
tc	702.71	K	Joback Method
tf	247.96	K	Joback Method
vc	0.706	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.67	J/mol×K	526.66	Joback Method
cpg	434.19	J/mol×K	556.00	Joback Method
cpg	448.99	J/mol×K	585.34	Joback Method
cpg	463.12	J/mol×K	614.69	Joback Method
cpg	476.60	J/mol×K	644.03	Joback Method
cpg	489.45	J/mol×K	673.37	Joback Method
cpg	501.71	J/mol×K	702.71	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13019164&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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