

2-n-Butylacrolein

Other names:	Hexanal, 2-methylene- 2-Butylacrolein 2-Methylene-hexanal
Inchi:	InChI=1S/C7H12O/c1-3-4-5-7(2)6-8/h6H,2-5H2,1H3
InchiKey:	IWEWQGKFUYQGSN-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	C=C(C=O)CCCC
Mol. weight [g/mol]:	112.17
CAS:	1070-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-12.17	kJ/mol	Joback Method
hf	-157.75	kJ/mol	Joback Method
hfus	13.58	kJ/mol	Joback Method
hvap	37.31	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1160.00		NIST Webbook
ripol	1160.00		NIST Webbook
tb	404.78	K	Joback Method
tc	583.47	K	Joback Method
tf	194.93	K	Joback Method
vc	0.426	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.95	J/molxK	404.78	Joback Method

cpg	212.54	J/mol×K	434.56	Joback Method
cpg	222.66	J/mol×K	464.34	Joback Method
cpg	232.34	J/mol×K	494.13	Joback Method
cpg	241.60	J/mol×K	523.91	Joback Method
cpg	250.43	J/mol×K	553.69	Joback Method
cpg	258.86	J/mol×K	583.47	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1070662&Units=SI

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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