(Z)-2-Butyloct-2-enal

Other names: 2-butyl-2-octenal (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: CCCCCC=C(C=O)CCCC
Mol. weight [g/mol]: 182.30

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
rinpol	1361.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
ripol	1688.00		NIST Webbook
tb	526.66	K	Joback Method
tc	702.71	K	Joback Method
tf	247.96	K	Joback Method
vc	0.706	m3/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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R282674&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
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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