2-Octenoic acid, 2-butyl

Inchi: InChI=1S/C12H22O2/c1-3-5-7-8-10-11(12(13)14)9-6-4-2/h10H,3-9H2,1-2H3,(H,13,14)/b1
InchiKey: DXAWUPPWNGZBOY-ZHACJKMWSA-N
Formula: C12H22O2
SMILES: CCCCCC=C(CCCC)C(=O)O
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-143.91	kJ/mol	Joback Method
hf	-448.39	kJ/mol	Joback Method
hfus	31.42	kJ/mol	Joback Method
hvap	65.77	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.768		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
tb	624.05	K	Joback Method
tc	797.54	K	Joback Method
tf	316.71	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.81	J/mol×K	624.05	Joback Method
cpg	495.22	J/mol×K	652.96	Joback Method
cpg	508.01	J/mol×K	681.88	Joback Method
cpg	520.20	J/mol×K	710.79	Joback Method
cpg	531.83	J/mol×K	739.71	Joback Method
cpg	542.91	J/mol×K	768.62	Joback Method
cpg	553.48	J/mol×K	797.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R54531&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume