4-Octen-1-ol, (Z)-, butanoate

Other names: (Z)-4-Octen-1-yl butanoate
Inchi: InChI=1S/C12H22O2/c1-3-5-6-7-8-9-11-14-12(13)10-4-2/h6-7H,3-5,8-11H2,1-2H3/b7-6-
InchiKey: ALDNKJSWCRXURS-SREVYHEPSA-N
Formula: C12H22O2
SMILES: CCCC=CCCCOC(=O)CCC
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-103.54	kJ/mol	Joback Method
hf	-418.59	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1354.00		NIST Webbook
tb	554.41	K	Joback Method
tc	730.90	K	Joback Method
tf	292.08	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.74	J/mol×K	554.41	Joback Method
cpg	461.06	J/mol×K	583.82	Joback Method
cpg	475.72	J/mol×K	613.24	Joback Method
cpg	489.74	J/mol×K	642.65	Joback Method

cpg	503.13	J/mol×K	672.07	Joback Method
cpg	515.92	J/mol×K	701.48	Joback Method
cpg	528.11	J/mol×K	730.90	Joback Method
dvisc	0.0028734	Pa×s	292.08	Joback Method
dvisc	0.0012967	Pa×s	335.80	Joback Method
dvisc	0.0007029	Pa×s	379.52	Joback Method
dvisc	0.0004324	Pa×s	423.25	Joback Method
dvisc	0.0002914	Pa×s	466.97	Joback Method
dvisc	0.0002101	Pa×s	510.69	Joback Method
dvisc	0.0001595	Pa×s	554.41	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R75660&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
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

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