3-Butenyl benzoate

Other names: 3-Buten-1-ol, benzoate
Inchi: InChI=1S/C11H12O2/c1-2-3-9-13-11(12)10-7-5-4-6-8-10/h2,4-8H,1,3,9H2
InchiKey: HCAQKYMCZZDLGU-UHFFFAOYSA-N
Formula: C11H12O2
SMILES: C=CCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 176.21

Physical Properties

Property code	Value	Unit	Source
gf	8.07	kJ/mol	Joback Method
hf	-153.21	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	50.84	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.420		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1337.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1334.00		NIST Webbook
ripol	1912.00		NIST Webbook
tb	550.73	K	Joback Method
tc	764.42	K	Joback Method
tf	310.55	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.91	J/mol×K	550.73	Joback Method
cpg	340.70	J/mol×K	586.34	Joback Method
cpg	353.66	J/mol×K	621.96	Joback Method
cpg	365.82	J/mol×K	657.57	Joback Method

cpg	377.21	J/mol×K	693.19	Joback Method
cpg	387.86	J/mol×K	728.80	Joback Method
cpg	397.79	J/mol×K	764.42	Joback Method
dvisc	0.0021881	Pa×s	310.55	Joback Method
dvisc	0.0011786	Pa×s	350.58	Joback Method
dvisc	0.0007207	Pa×s	390.61	Joback Method
dvisc	0.0004829	Pa×s	430.64	Joback Method
dvisc	0.0003463	Pa×s	470.67	Joback Method
dvisc	0.0002617	Pa×s	510.70	Joback Method
dvisc	0.0002060	Pa×s	550.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30951&Units=SI

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