(E)-2-Butenyl benzoate

Inchi: InChI=1S/C11H12O2/c1-2-3-9-13-11(12)10-7-5-4-6-8-10/h2-8H,9H2,1H3/b3-2+
InchiKey: QYOVCBKZFRCMCG-NSCUHMNNSA-N
Formula: C11H12O2
SMILES: CC=CCOC(=O)c1ccccc1
Mol. weight [g/mol]: 176.21

Physical Properties

Property code	Value	Unit	Source
gf	0.45	kJ/mol	Joback Method
hf	-161.42	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	51.47	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.420		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1369.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1371.00		NIST Webbook
ripol	1973.00		NIST Webbook
ripol	1931.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1931.00		NIST Webbook
ripol	1986.00		NIST Webbook
ripol	1951.00		NIST Webbook

ripol	1956.00		NIST Webbook
tb	558.21	K	Joback Method
tc	776.95	K	Joback Method
tf	307.23	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.27	J/mol×K	558.21	Joback Method
cpg	341.18	J/mol×K	594.67	Joback Method
cpg	354.22	J/mol×K	631.12	Joback Method
cpg	366.41	J/mol×K	667.58	Joback Method
cpg	377.80	J/mol×K	704.04	Joback Method
cpg	388.43	J/mol×K	740.50	Joback Method
cpg	398.33	J/mol×K	776.95	Joback Method
dvisc	0.0021241	Pa×s	307.23	Joback Method
dvisc	0.0010842	Pa×s	349.06	Joback Method
dvisc	0.0006391	Pa×s	390.89	Joback Method
dvisc	0.0004172	Pa×s	432.72	Joback Method
dvisc	0.0002937	Pa×s	474.55	Joback Method
dvisc	0.0002188	Pa×s	516.38	Joback Method
dvisc	0.0001704	Pa×s	558.21	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R30933&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume