benzyl (E)-2-butenoate

Other names: Benzyl crotonate
benzyl but-2-enoate
benzyl crotane
Inchi: InChI=1S/C11H12O2/c1-2-6-11(12)13-9-10-7-4-3-5-8-10/h2-8H,9H2,1H3/b6-2+
InchiKey: NCPTYZLUYHXITE-QHHAFSJGSA-N
Formula: C11H12O2
SMILES: CC=CC(=O)OCc1ccccc1
Mol. weight [g/mol]: 176.21
CAS: 65416-24-2

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	-2.74		Crippen Method
logp	2.306		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1396.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1396.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	2020.00		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

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=C65416242&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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