Benzoic acid, 2-propenyl ester

Other names:	Benzoic acid, allyl ester
	Allyl benzoate
	2-Propenyl benzoate
Inchi:	InChI=1S/C10H10O2/c1-2-8-12-10(11)9-6-4-3-5-7-9/h2-7H,1,8H2
InchiKey:	LYJHVEDILOKZCG-UHFFFAOYSA-N
Formula:	C10H10O2
SMILES:	C=CCOC(=O)c1ccccc1
Mol. weight [g/mol]:	162.19
CAS:	583-04-0

Physical Properties

Property code	Value	Unit	Source
gf	-0.35	kJ/mol	Joback Method
hf	-132.57	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	48.62	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.029		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	1248.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1241.00		NIST Webbook

rinpol	1230.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1802.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1848.00		NIST Webbook
ripol	1834.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1836.00		NIST Webbook
tb	502.90 ± 1.50	K	NIST Webbook
tc	745.16	K	Joback Method
tf	299.28	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.78	J/mol×K	527.85	Joback Method
cpg	294.67	J/mol×K	564.07	Joback Method
cpg	306.78	J/mol×K	600.29	Joback Method
cpg	318.13	J/mol×K	636.51	Joback Method
cpg	328.76	J/mol×K	672.73	Joback Method
cpg	338.67	J/mol×K	708.94	Joback Method
cpg	347.91	J/mol×K	745.16	Joback Method
dvisc	0.0022001	Pa×s	299.28	Joback Method
dvisc	0.0012082	Pa×s	337.38	Joback Method
dvisc	0.0007493	Pa×s	375.47	Joback Method
dvisc	0.0005075	Pa×s	413.56	Joback Method
dvisc	0.0003670	Pa×s	451.66	Joback Method
dvisc	0.0002792	Pa×s	489.75	Joback Method
dvisc	0.0002209	Pa×s	527.85	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=C583040&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