1-Phenyl-1-butene

Other names: Benzene, 1-butenyl
«beta»-Ethylstyrene
1-Butenyl-benzene
Inchi: InChI=1S/C10H12/c1-2-3-7-10-8-5-4-6-9-10/h3-9H,2H2,1H3
InchiKey: MPMBRWOOISTHJV-UHFFFAOYSA-N
Formula: C10H12
SMILES: CCC=Cc1ccccc1
Mol. weight [g/mol]: 132.20
CAS: 824-90-8

Physical Properties

Property code	Value	Unit	Source
chl	-5639.60	kJ/mol	NIST Webbook
gf	225.95	kJ/mol	Joback Method
hf	104.02	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	40.09	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.110		Crippen Method
mcvol	123.700	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1098.20		NIST Webbook
rinpol	1112.00		NIST Webbook
tb	462.15 ± 2.00	K	NIST Webbook
tb	453.15 ± 2.00	K	NIST Webbook
tb	450.00 ± 5.00	K	NIST Webbook
tb	471.83 ± 0.30	K	NIST Webbook
tb	471.83 ± 0.50	K	NIST Webbook
tb	470.15 ± 2.00	K	NIST Webbook
tc	673.98	K	Joback Method
tf	230.09 ± 0.50	K	NIST Webbook
tf	230.09 ± 0.20	K	NIST Webbook
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.15	J/mol×K	459.04	Joback Method
cpg	254.92	J/mol×K	494.86	Joback Method
cpg	268.75	J/mol×K	530.69	Joback Method
cpg	281.69	J/mol×K	566.51	Joback Method
cpg	293.79	J/mol×K	602.33	Joback Method
cpg	305.09	J/mol×K	638.16	Joback Method
cpg	315.65	J/mol×K	673.98	Joback Method
dvisc	0.0034135	Pa×s	223.80	Joback Method
dvisc	0.0014730	Pa×s	263.01	Joback Method
dvisc	0.0007906	Pa×s	302.21	Joback Method
dvisc	0.0004895	Pa×s	341.42	Joback Method
dvisc	0.0003345	Pa×s	380.63	Joback Method
dvisc	0.0002455	Pa×s	419.83	Joback Method
dvisc	0.0001899	Pa×s	459.04	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=C824908&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
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