

(E)-4-Phenylbut-3-en-2-ol

Inchi: InChI=1S/C10H12O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-9,11H,1H3/b8-7+
InchiKey: ZIJWGEHOVHJHKB-BQYQJAHWSA-N
Formula: C10H12O
SMILES: CC(O)C=Cc1ccccc1
Mol. weight [g/mol]: 148.20

Physical Properties

Property code	Value	Unit	Source
gf	86.69	kJ/mol	Joback Method
hf	-53.49	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	56.38	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.081		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	1315.00		NIST Webbook
tb	550.78	K	Joback Method
tc	755.82	K	Joback Method
tf	269.62	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.06	J/mol×K	550.78	Joback Method
cpg	347.04	J/mol×K	721.65	Joback Method
cpg	337.63	J/mol×K	687.48	Joback Method
cpg	327.57	J/mol×K	653.30	Joback Method
cpg	316.82	J/mol×K	619.13	Joback Method
cpg	305.33	J/mol×K	584.95	Joback Method
cpg	355.85	J/mol×K	755.82	Joback Method
dvisc	0.0000833	Pa×s	550.78	Joback Method
dvisc	0.0001387	Pa×s	503.92	Joback Method

dvisc	0.0002564	Pa×s	457.06	Joback Method
dvisc	0.0005452	Pa×s	410.20	Joback Method
dvisc	0.0014087	Pa×s	363.34	Joback Method
dvisc	0.0048211	Pa×s	316.48	Joback Method
dvisc	0.0253050	Pa×s	269.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341283&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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