

Benzene, 4-(2-butenyl)-1,2-dimethyl-, (E)-

Inchi:	InChI=1S/C12H16/c1-4-5-6-12-8-7-10(2)11(3)9-12/h4-5,7-9H,6H2,1-3H3/b5-4+
InchiKey:	PKDQZBULDXXKDSQ-SNAWJCMRSA-N
Formula:	C12H16
SMILES:	CC=CCc1ccc(C)c(C)c1
Mol. weight [g/mol]:	160.26
CAS:	54340-86-2

Physical Properties

Property code	Value	Unit	Source
gf	223.53	kJ/mol	Joback Method
hf	39.80	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	45.86	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.422		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
tb	514.76	K	Joback Method
tc	725.81	K	Joback Method
tf	271.38	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.21	J/molxK	514.76	Joback Method
cpg	344.98	J/molxK	549.93	Joback Method
cpg	359.86	J/molxK	585.11	Joback Method
cpg	373.91	J/molxK	620.28	Joback Method
cpg	387.16	J/molxK	655.46	Joback Method
cpg	399.66	J/molxK	690.63	Joback Method
cpg	411.44	J/molxK	725.81	Joback Method
dvisc	0.0017124	Paxs	271.38	Joback Method
dvisc	0.0008978	Paxs	311.94	Joback Method

dvisc	0.0005462	Paxs	352.51	Joback Method
dvisc	0.0003681	Paxs	393.07	Joback Method
dvisc	0.0002671	Paxs	433.63	Joback Method
dvisc	0.0002048	Paxs	474.20	Joback Method
dvisc	0.0001637	Paxs	514.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54340862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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