

2-Phenoxy-3-methyl-2-butene

Inchi:	InChI=1S/C11H14O/c1-9(2)10(3)12-11-7-5-4-6-8-11/h4-8H,1-3H3
InchiKey:	DYDDSAIUIFYQRNP-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CC(C)=C(C)Oc1ccccc1
Mol. weight [g/mol]:	162.23
CAS:	42237-97-8

Physical Properties

Property code	Value	Unit	Source
gf	112.27	kJ/mol	Joback Method
hf	-68.42	kJ/mol	Joback Method
hfus	17.06	kJ/mol	Joback Method
hvap	44.88	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.379		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
tb	504.10	K	Joback Method
tc	722.22	K	Joback Method
tf	229.38	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.91	J/mol×K	504.10	Joback Method
cpg	323.66	J/mol×K	540.45	Joback Method
cpg	338.47	J/mol×K	576.81	Joback Method
cpg	352.38	J/mol×K	613.16	Joback Method
cpg	365.44	J/mol×K	649.51	Joback Method
cpg	377.69	J/mol×K	685.87	Joback Method
cpg	389.17	J/mol×K	722.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C42237978&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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