2-Isopropoxy-3-methyl-1-butene

Inchi: InChI=1S/C8H16O/c1-6(2)8(5)9-7(3)4/h6-7H,5H2,1-4H3
InchiKey: NJQBVLZZZOURKA-UHFFFAOYSA-N
Formula: C8H16O
SMILES: C=C(OC(C)C)C(C)C
Mol. weight [g/mol]: 128.21
CAS: 56544-18-4

Physical Properties

Property code	Value	Unit	Source
gf	-14.11	kJ/mol	Joback Method
hf	-235.59	kJ/mol	Joback Method
hfus	8.03	kJ/mol	Joback Method
hvap	34.45	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.581		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
tb	400.54	K	Joback Method
tc	578.95	K	Joback Method
tf	156.43	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.18	J/mol×K	400.54	Joback Method
cpg	255.29	J/mol×K	430.27	Joback Method
cpg	267.93	J/mol×K	460.01	Joback Method
cpg	280.10	J/mol×K	489.74	Joback Method
cpg	291.80	J/mol×K	519.48	Joback Method
cpg	303.04	J/mol×K	549.21	Joback Method
cpg	313.84	J/mol×K	578.95	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=C56544184&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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