1-(4-Isobutylphenyl)-1-ethanol, methyl

Inchi: InChI=1S/C13H20O/c1-10(2)9-12-5-7-13(8-6-12)11(3)14-4/h5-8,10-11H,9H2,1-4H3
InchiKey: CXJYXHFRLZJNKT-UHFFFAOYSA-N
Formula: C13H20O
SMILES: COC(C)c1ccc(CC(C)C)cc1
Mol. weight [g/mol]: 192.30

Physical Properties

Property code	Value	Unit	Source
gf	51.48	kJ/mol	Joback Method
hf	-229.37	kJ/mol	Joback Method
hfus	17.22	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.593		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	1322.00		NIST Webbook
rinpol	1322.00		NIST Webbook
tb	550.04	K	Joback Method
tc	754.44	K	Joback Method
tf	267.44	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.06	J/mol×K	550.04	Joback Method
cpg	500.58	J/mol×K	720.37	Joback Method
cpg	486.39	J/mol×K	686.31	Joback Method
cpg	471.37	J/mol×K	652.24	Joback Method
cpg	455.49	J/mol×K	618.17	Joback Method
cpg	438.73	J/mol×K	584.11	Joback Method
cpg	513.94	J/mol×K	754.44	Joback Method
dvisc	0.0001368	Pa×s	550.04	Joback Method

dvisc	0.0001832	Pa×s	502.94	Joback Method
dvisc	0.0002605	Pa×s	455.84	Joback Method
dvisc	0.0004018	Pa×s	408.74	Joback Method
dvisc	0.0006938	Pa×s	361.64	Joback Method
dvisc	0.0014111	Pa×s	314.54	Joback Method
dvisc	0.0036850	Pa×s	267.44	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=R399465&Units=SI

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