«alpha»-methyl-3-(1-methylethyl)benzeneethanol

Inchi: InChI=1S/C12H18O/c1-9(2)12-6-4-5-11(8-12)7-10(3)13/h4-6,8-10,13H,7H2,1-3H3
InchiKey: PTCONCVHDYBONT-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC(O)Cc1cccc(C(C)C)c1
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	11.24	kJ/mol	Joback Method
hf	-228.74	kJ/mol	Joback Method
hfus	17.53	kJ/mol	Joback Method
hvap	61.15	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.733		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
ripol	1918.00		NIST Webbook
ripol	1918.00		NIST Webbook
tb	596.92	K	Joback Method
tc	792.94	K	Joback Method
tf	294.76	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.35	J/mol×K	596.92	Joback Method
cpg	471.38	J/mol×K	760.27	Joback Method
cpg	460.01	J/mol×K	727.60	Joback Method
cpg	447.95	J/mol×K	694.93	Joback Method
cpg	435.17	J/mol×K	662.26	Joback Method
cpg	421.65	J/mol×K	629.59	Joback Method
cpg	482.09	J/mol×K	792.94	Joback Method
dvisc	0.0000644	Pa×s	596.92	Joback Method

dvisc	0.0001058	Pa×s	546.56	Joback Method
dvisc	0.0001922	Pa×s	496.20	Joback Method
dvisc	0.0003999	Pa×s	445.84	Joback Method
dvisc	0.0010024	Pa×s	395.48	Joback Method
dvisc	0.0032859	Pa×s	345.12	Joback Method
dvisc	0.0161608	Pa×s	294.76	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=R321170&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume