d-methyl-tert-butylcarbinol

Inchi: InChI=1S/C6H14O/c1-5(7)6(2,3)4/h5,7H,1-4H3/t5-/m1/s1
InchiKey: DFOXKPDFWGNLJU-RXMQYKEDSA-N
Formula: C6H14O
SMILES: CC(O)C(C)(C)C
Mol. weight [g/mol]: 102.17
CAS: 1517-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-136.78	kJ/mol	Joback Method
hf	-333.43	kJ/mol	Joback Method
hfus	4.45	kJ/mol	Joback Method
hvap	43.95	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.413		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	393.20 ± 2.00	K	NIST Webbook
tb	392.65 ± 2.00	K	NIST Webbook
tc	600.02	K	Joback Method
tf	205.62	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.06	J/mol×K	425.19	Joback Method
cpg	220.98	J/mol×K	454.33	Joback Method
cpg	231.37	J/mol×K	483.47	Joback Method
cpg	241.24	J/mol×K	512.60	Joback Method
cpg	250.62	J/mol×K	541.74	Joback Method
cpg	259.53	J/mol×K	570.88	Joback Method
cpg	267.98	J/mol×K	600.02	Joback Method
dvisc	0.3533787	Pa×s	205.62	Joback Method

dvisc	0.0427885	Pa×s	242.22	Joback Method
dvisc	0.0090180	Pa×s	278.81	Joback Method
dvisc	0.0027278	Pa×s	315.40	Joback Method
dvisc	0.0010580	Pa×s	352.00	Joback Method
dvisc	0.0004905	Pa×s	388.60	Joback Method
dvisc	0.0002596	Pa×s	425.19	Joback Method

Sources

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=C1517675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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