1-Pentanol, 3-methyl-, (.+/-.)-

Inchi: InChI=1S/C6H14O/c1-3-6(2)4-5-7/h6-7H,3-5H2,1-2H3
InchiKey: IWTBVKIGCDZRPL-UHFFFAOYSA-N
Formula: C6H14O
SMILES: CCC(C)CCO
Mol. weight [g/mol]: 102.17
CAS: 20281-83-8

Physical Properties

Property code	Value	Unit	Source
gf	-139.62	kJ/mol	Joback Method
hf	-324.68	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	45.24	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.415		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	426.20	K	NIST Webbook
tc	592.97	K	Joback Method
tf	203.20	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.74	J/mol×K	428.42	Joback Method
cpg	253.18	J/mol×K	565.55	Joback Method
cpg	244.78	J/mol×K	538.12	Joback Method
cpg	236.05	J/mol×K	510.70	Joback Method
cpg	226.97	J/mol×K	483.27	Joback Method
cpg	217.54	J/mol×K	455.85	Joback Method
cpg	261.25	J/mol×K	592.97	Joback Method
dvisc	0.0002400	Pa×s	428.42	Joback Method
dvisc	0.0004330	Pa×s	390.88	Joback Method

dvisc	0.0008856	Pa×s	353.35	Joback Method
dvisc	0.0021472	Pa×s	315.81	Joback Method
dvisc	0.0066108	Pa×s	278.27	Joback Method
dvisc	0.0289027	Pa×s	240.74	Joback Method
dvisc	0.2179366	Pa×s	203.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	325.20	K	1.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20281838&Units=SI
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

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume