Threo-3-methylpentan-2-ol

Inchi: InChI=1S/C6H14O/c1-4-5(2)6(3)7/h5-7H,4H2,1-3H3/t5-,6-/m1/s1
InchiKey: ZXNBBWHRUSXUFZ-PHDIDXHHSA-N
Formula: C6H14O
SMILES: CCC(C)C(C)O
Mol. weight [g/mol]: 102.17
CAS: 1502-93-8

Physical Properties

Property code	Value	Unit	Source
gf	-142.06	kJ/mol	Joback Method
hf	-329.96	kJ/mol	Joback Method
hfus	8.34	kJ/mol	Joback Method
hvap	44.85	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.413		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
tb	427.98	K	Joback Method
tc	596.11	K	Joback Method
tf	188.20	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.81	J/mol×K	427.98	Joback Method
cpg	254.50	J/mol×K	568.09	Joback Method
cpg	245.89	J/mol×K	540.06	Joback Method
cpg	236.93	J/mol×K	512.04	Joback Method
cpg	227.60	J/mol×K	484.02	Joback Method
cpg	217.90	J/mol×K	456.00	Joback Method
cpg	262.76	J/mol×K	596.11	Joback Method
dvisc	0.0002307	Pa×s	427.98	Joback Method
dvisc	0.0004388	Pa×s	388.02	Joback Method

dvisc	0.0009671	Pa×s	348.05	Joback Method
dvisc	0.0026164	Pa×s	308.09	Joback Method
dvisc	0.0095238	Pa×s	268.13	Joback Method
dvisc	0.0545090	Pa×s	228.16	Joback Method
dvisc	0.6544822	Pa×s	188.20	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=C1502938&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