

2,5-Dihydroxyheptane

Inchi:	InChI=1S/C7H16O2/c1-3-7(9)5-4-6(2)8/h6-9H,3-5H2,1-2H3
InchiKey:	XTVHTJKQKUOEQA-UHFFFAOYSA-N
Formula:	C7H16O2
SMILES:	CCC(O)CCC(C)O
Mol. weight [g/mol]:	132.20
CAS:	70444-25-6

Physical Properties

Property code	Value	Unit	Source
gf	-270.46	kJ/mol	Joback Method
hf	-502.83	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	63.76	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.918		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	543.04	K	Joback Method
tc	705.35	K	Joback Method
tf	260.29	K	Joback Method
vc	0.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.72	J/molxK	543.04	Joback Method
cpg	309.47	J/molxK	570.09	Joback Method
cpg	318.84	J/molxK	597.14	Joback Method
cpg	327.82	J/molxK	624.19	Joback Method
cpg	336.43	J/molxK	651.24	Joback Method
cpg	344.68	J/molxK	678.30	Joback Method
cpg	352.58	J/molxK	705.35	Joback Method
dvisc	0.4213623	Paxs	260.29	Joback Method
dvisc	0.0300384	Paxs	307.42	Joback Method

dvisc	0.0043212	Paxs	354.54	Joback Method
dvisc	0.0009798	Paxs	401.66	Joback Method
dvisc	0.0003034	Paxs	448.79	Joback Method
dvisc	0.0001174	Paxs	495.91	Joback Method
dvisc	0.0000536	Paxs	543.04	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=C70444256&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

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