

1-Heptanol, 2-propyl-

Other names:	2-Propylheptanol 2-propylheptan-1-ol
Inchi:	InChI=1S/C10H22O/c1-3-5-6-8-10(9-11)7-4-2/h10-11H,3-9H2,1-2H3
InchiKey:	YLQLIQIAXYRMDL-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCCCCC(CO)CCC
Mol. weight [g/mol]:	158.28
CAS:	10042-59-8

Physical Properties

Property code	Value	Unit	Source
gf	-105.94	kJ/mol	Joback Method
hf	-407.24	kJ/mol	Joback Method
hfus	22.22	kJ/mol	Joback Method
hvap	54.14	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.975		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
tb	519.94	K	Joback Method
tc	681.25	K	Joback Method
tf	248.28	K	Joback Method
vc	0.609	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.84	J/mol×K	519.94	Joback Method
cpg	394.36	J/mol×K	546.83	Joback Method
cpg	407.36	J/mol×K	573.71	Joback Method
cpg	419.85	J/mol×K	600.60	Joback Method
cpg	431.84	J/mol×K	627.48	Joback Method
cpg	443.35	J/mol×K	654.37	Joback Method
cpg	454.40	J/mol×K	681.25	Joback Method

dvisc	0.0660457	Paxs	248.28	Joback Method
dvisc	0.0101842	Paxs	293.56	Joback Method
dvisc	0.0025882	Paxs	338.83	Joback Method
dvisc	0.0009085	Paxs	384.11	Joback Method
dvisc	0.0003977	Paxs	429.39	Joback Method
dvisc	0.0002038	Paxs	474.66	Joback Method
dvisc	0.0001173	Paxs	519.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C10042598&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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