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	m3/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	Pa×s	248.28	Joback Method
dvisc	0.0101842	Pa×s	293.56	Joback Method
dvisc	0.0025882	Pa×s	338.83	Joback Method
dvisc	0.0009085	Pa×s	384.11	Joback Method
dvisc	0.0003977	Pa×s	429.39	Joback Method
dvisc	0.0002038	Pa×s	474.66	Joback Method
dvisc	0.0001173	Pa×s	519.94	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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