n-Propyl heptyl ether

Other names: Heptyl propyl ether
Inchi: InChI=1S/C10H22O/c1-3-5-6-7-8-10-11-9-4-2/h3-10H2,1-2H3
InchiKey: DOYXDCAHTUMXDF-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CCCCCCCOCCC
Mol. weight [g/mol]: 158.28
CAS: 71112-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-71.68	kJ/mol	Joback Method
hf	-381.95	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	40.26	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.383		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	1075.00		NIST Webbook
rinpol	1075.00		NIST Webbook
tb	450.62	K	Joback Method
tc	613.22	K	Joback Method
tf	224.69	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.40	J/mol×K	450.62	Joback Method
cpg	411.42	J/mol×K	586.12	Joback Method
cpg	398.57	J/mol×K	559.02	Joback Method
cpg	385.25	J/mol×K	531.92	Joback Method
cpg	371.45	J/mol×K	504.82	Joback Method
cpg	357.17	J/mol×K	477.72	Joback Method

cpg	423.80	J/mol×K	613.22	Joback Method
dvisc	0.0002026	Pa×s	450.62	Joback Method
dvisc	0.0002676	Pa×s	412.97	Joback Method
dvisc	0.0003736	Pa×s	375.31	Joback Method
dvisc	0.0005620	Pa×s	337.65	Joback Method
dvisc	0.0009367	Pa×s	300.00	Joback Method
dvisc	0.0018076	Pa×s	262.35	Joback Method
dvisc	0.0043485	Pa×s	224.69	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=C71112895&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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