

Propane, 2-methyl-1-propoxy-

Inchi:	InChI=1S/C7H16O/c1-4-5-8-6-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	NKBWHRMIYKMDDN-UHFFFAOYSA-N
Formula:	C7H16O
SMILES:	CCCOCC(C)C
Mol. weight [g/mol]:	116.20
CAS:	15268-49-2

Physical Properties

Property code	Value	Unit	Source
gf	-99.38	kJ/mol	Joback Method
hf	-325.31	kJ/mol	Joback Method
hfus	11.55	kJ/mol	Joback Method
hvap	38.25	kJ/mol	NIST Webbook
log10ws	-1.60		Crippen Method
logp	2.069		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	381.00	K	NIST Webbook
tc	549.69	K	Joback Method
tf	175.88	K	Joback Method
vc	0.440	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.33	J/molxK	381.54	Joback Method
cpg	230.17	J/molxK	409.57	Joback Method
cpg	241.65	J/molxK	437.59	Joback Method
cpg	252.77	J/molxK	465.62	Joback Method
cpg	263.53	J/molxK	493.64	Joback Method
cpg	273.94	J/molxK	521.67	Joback Method
cpg	284.00	J/molxK	549.69	Joback Method
dvisc	0.0068890	Paxs	175.88	Joback Method
dvisc	0.0024170	Paxs	210.16	Joback Method

dvisc	0.0011375	Paxs	244.43	Joback Method
dvisc	0.0006444	Paxs	278.71	Joback Method
dvisc	0.0004135	Paxs	312.99	Joback Method
dvisc	0.0002896	Paxs	347.26	Joback Method
dvisc	0.0002162	Paxs	381.54	Joback Method
hvapt	32.55	kJ/mol	381.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.70	K	96.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15268492&Units=SI
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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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