ISOBUTYL-PROPYL-AMINE

Other names: (2-Methyl-n-propyl)-1-propanamine
Propylisobutylamine
N-Isobutyl-N-propylamine
isobutyl-n-propyl-amine
Inchi: InChI=1S/C7H17N/c1-4-5-8-6-7(2)3/h7-8H,4-6H2,1-3H3
InchiKey: SQGSVBHTFQOZDL-UHFFFAOYSA-N
Formula: C7H17N
SMILES: CCCNCC(C)C
Mol. weight [g/mol]: 115.22

Physical Properties

Property code	Value	Unit	Source
af	0.4254		Cheméo Relay (1.0)
hf	-145.97	kJ/mol	Cheméo Relay (1.0)
hfus	15.46	kJ/mol	Joback Method
hvap	39.81	kJ/mol	Cheméo Relay (1.0)
ie	7.95	eV	Cheméo Relay (1.0)
log10ws	-1.14		Cheméo Relay (1.0)
logp	1.642		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	797.00		NIST Webbook
rinpol	797.00		NIST Webbook
ripol	918.00		NIST Webbook
ripol	918.00		NIST Webbook
tb	397.15 ± 2.00	K	NIST Webbook
tc	540.01	K	Cheméo Relay (1.0)
tf	189.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.14	J/mol×K	409.29	Joback Method
cpg	251.08	J/mol×K	438.13	Joback Method

cpg	263.53	J/mol×K	466.97	Joback Method
cpg	275.48	J/mol×K	495.82	Joback Method
cpg	286.96	J/mol×K	524.66	Joback Method
cpg	297.97	J/mol×K	553.50	Joback Method
cpg	308.53	J/mol×K	582.34	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39190664&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point