

isoamylethyl-amine

Inchi:	InChI=1S/C7H17N/c1-4-8-6-5-7(2)3/h7-8H,4-6H2,1-3H3
InchiKey:	TZTQUOTYYSUZNA-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CCNCCC(C)C
Mol. weight [g/mol]:	115.22
CAS:	21035-52-9

Physical Properties

Property code	Value	Unit	Source
gf	95.01	kJ/mol	Joback Method
hf	-139.62	kJ/mol	Joback Method
hfus	15.46	kJ/mol	Joback Method
hvap	37.22	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.642		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	821.00		NIST Webbook
tb	409.29	K	Joback Method
tc	582.34	K	Joback Method
tf	206.31	K	Joback Method
vc	0.457	m3/kmol	Joback Method

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21035529&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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