2-methyl-1-pentanamine

Other names: 2-methyl-1-pentanamine
Inchi: InChI=1S/C6H15N/c1-3-4-6(2)5-7/h6H,3-5,7H2,1-2H3
InchiKey: WNDXRJBYZOSNQO-UHFFFAOYSA-N
Formula: C6H15N
SMILES: CCCC(C)CN
Mol. weight [g/mol]: 101.19

Physical Properties

Property code	Value	Unit	Source
af	0.4088		Cheméo Relay (1.0)
gf	63.65	kJ/mol	Joback Method
hf	-164.79	kJ/mol	Cheméo Relay (1.0)
hfus	12.97	kJ/mol	Joback Method
hvap	40.55	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
log10ws	-1.45		Cheméo Relay (1.0)
logp	1.381		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	394.83	K	Cheméo Relay (1.0)
tc	567.23	K	Cheméo Relay (1.0)
tf	202.78	K	Cheméo Relay (1.0)
vc	0.364	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.01	J/mol×K	408.77	Joback Method
cpg	222.78	J/mol×K	439.46	Joback Method
cpg	234.07	J/mol×K	470.15	Joback Method
cpg	244.89	J/mol×K	500.84	Joback Method
cpg	255.25	J/mol×K	531.53	Joback Method
cpg	265.17	J/mol×K	562.22	Joback Method
cpg	274.66	J/mol×K	592.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13364164&Units=SI
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):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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