Pentanoic acid, 4-methyl-2-methylamino, methyl ester

Inchi: InChI=1S/C8H17NO2/c1-6(2)5-7(9-3)8(10)11-4/h6-7,9H,5H2,1-4H3
InchiKey: NYXMJFGTJZTHPT-UHFFFAOYSA-N
Formula: C8H17NO2
SMILES: CNC(CC(C)C)C(=O)OC
Mol. weight [g/mol]: 159.23

Physical Properties

Property code	Value	Unit	Source
gf	-132.93	kJ/mol	Joback Method
hf	-410.34	kJ/mol	Joback Method
hfus	17.32	kJ/mol	Joback Method
hvap	48.22	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	0.793		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	1014.00		NIST Webbook
rinpol	1014.00		NIST Webbook
tb	508.02	K	Joback Method
tc	693.40	K	Joback Method
tf	274.74	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.33	J/mol×K	508.02	Joback Method
cpg	340.70	J/mol×K	538.92	Joback Method
cpg	353.51	J/mol×K	569.81	Joback Method
cpg	365.78	J/mol×K	600.71	Joback Method
cpg	377.51	J/mol×K	631.61	Joback Method
cpg	388.70	J/mol×K	662.51	Joback Method
cpg	399.36	J/mol×K	693.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R106713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume