Propanamide, 2,2-dimethyl-

Other names:	2,2-dimethylpropanamide
	Trimethylacetamide
	pivalamide
Inchi:	InChI=1S/C5H11NO/c1-5(2,3)4(6)7/h1-3H3,(H2,6,7)
InchiKey:	XIPFMBOWZXULIA-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CC(C)(C)C(N)=O
Mol. weight [g/mol]:	101.15
CAS:	754-10-9

Physical Properties

Property code	Value	Unit	Source
affp	889.00	kJ/mol	NIST Webbook
basg	857.20	kJ/mol	NIST Webbook
basg	855.00 ± 6.00	kJ/mol	NIST Webbook
basg	858.00 ± 7.00	kJ/mol	NIST Webbook
chs	-3139.90 ± 1.20	kJ/mol	NIST Webbook
gf	-68.41	kJ/mol	Joback Method
hf	-313.10 ± 1.40	kJ/mol	NIST Webbook
hfs	-399.70 ± 1.30	kJ/mol	NIST Webbook
hfus	24.10	kJ/mol	Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry
hsub	89.00 ± 2.00	kJ/mol	NIST Webbook
hsub	86.60 ± 0.40	kJ/mol	NIST Webbook
hsub	86.60 ± 0.40	kJ/mol	NIST Webbook
hvap	42.81	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.518		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
tb	485.20	K	NIST Webbook
tc	643.53	K	Joback Method
tf	281.72	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.03	J/mol×K	436.97	Joback Method
cpg	202.71	J/mol×K	471.40	Joback Method
cpg	212.75	J/mol×K	505.82	Joback Method
cpg	222.17	J/mol×K	540.25	Joback Method
cpg	231.01	J/mol×K	574.68	Joback Method
cpg	239.29	J/mol×K	609.11	Joback Method
cpg	247.05	J/mol×K	643.53	Joback Method
cpl	159.80	J/mol×K	298.15	NIST Webbook
hfust	24.10	kJ/mol	425.40	NIST Webbook
hsubt	86.60	kJ/mol	298.15	NIST Webbook
ssubt	290.50	J/mol×K	298.15	NIST Webbook

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=C754109&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat Capacities and Enthalpies of Solid-Solid Transitions and Fusion of a Series of Eleven Primary Alkylamides by Differential Scanning Calorimetry:	https://www.doi.org/10.1021/je700662a

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
ssubt:	Entropy of sublimation at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume