Butenamide, N,N-dimethyl-

Other names: But-2-enamide, N,N-dimethyl-
Inchi: InChI=1S/C6H11NO/c1-4-5-6(8)7(2)3/h4-5H,1-3H3/b5-4+
InchiKey: VPFXWMDVXYAJGV-SNAWJCMRSA-N
Formula: C6H11NO
SMILES: CC=CC(=O)N(C)C
Mol. weight [g/mol]: 113.16
CAS: 23135-18-4

Physical Properties

Property code	Value	Unit	Source
affp	930.30	kJ/mol	NIST Webbook
basg	899.40	kJ/mol	NIST Webbook
gf	61.72	kJ/mol	Joback Method
hf	-95.00	kJ/mol	Joback Method
hfus	16.12	kJ/mol	Joback Method
hvap	37.70	kJ/mol	Joback Method
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-0.53		Crippen Method
logp	0.651		Crippen Method
mcvol	102.650	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	407.15	K	Joback Method
tc	592.16	K	Joback Method
tf	234.70	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.31	J/mol×K	407.15	Joback Method
cpg	201.31	J/mol×K	437.99	Joback Method
cpg	211.74	J/mol×K	468.82	Joback Method
cpg	221.61	J/mol×K	499.66	Joback Method
cpg	230.96	J/mol×K	530.49	Joback Method

cpg	239.81	J/mol×K	561.33	Joback Method
cpg	248.18	J/mol×K	592.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23135184&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

affp:	Proton affinity
basg:	Gas basicity
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