Butanamide, N,N-diethyl-3-oxo-

Other names:	Acetoacetamide, N,N-diethyl-
	Diethylacetoacetamide
	N,N-Diethylacetoacetamide
	1-(Diethylcarbamoyl)-2-propanone
	Acetoacetdiethylamide
	Diethylamid kyseliny acetoctove
	N,N-diethyl-3-oxobutyramide
Inchi:	InChI=1S/C8H15NO2/c1-4-9(5-2)8(11)6-7(3)10/h4-6H2,1-3H3
InchiKey:	NTMXFHGYWJIAAE-UHFFFAOYSA-N
Formula:	C8H15NO2
SMILES:	CCN(CC)C(=O)CC(C)=O
Mol. weight [g/mol]:	157.21
CAS:	2235-46-3

Physical Properties

Property code	Value	Unit	Source
gf	-130.58	kJ/mol	Joback Method
hf	-366.08	kJ/mol	Joback Method
hfus	22.70	kJ/mol	Joback Method
hvap	48.94	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.834		Crippen Method
mcvol	136.700	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
tb	502.62	K	Joback Method
tc	686.30	K	Joback Method
tf	312.25	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.89	J/mol×K	502.62	Joback Method
cpg	320.47	J/mol×K	533.23	Joback Method

cpg	332.45	J/mol×K	563.85	Joback Method
cpg	343.84	J/mol×K	594.46	Joback Method
cpg	354.67	J/mol×K	625.08	Joback Method
cpg	364.94	J/mol×K	655.69	Joback Method
cpg	374.69	J/mol×K	686.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2235463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume