Acetoacetamide, n-tert-butyl-

Inchi: InChI=1S/C8H15NO2/c1-6(10)5-7(11)9-8(2,3)4/h5H2,1-4H3,(H,9,11)
InchiKey: CGGJVHBWBNSMLY-UHFFFAOYSA-N
Formula: C8H15NO2
SMILES: CC(=O)CC(=O)NC(C)(C)C
Mol. weight [g/mol]: 157.21
CAS: 42222-06-0

Physical Properties

Property code	Value	Unit	Source
gf	-149.13	kJ/mol	Joback Method
hf	-388.89	kJ/mol	Joback Method
hfus	17.36	kJ/mol	Joback Method
hvap	52.03	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	0.880		Crippen Method
mcvol	136.700	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	537.12	K	Joback Method
tc	736.00	K	Joback Method
tf	334.86	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.87	J/mol×K	537.12	Joback Method
cpg	337.73	J/mol×K	570.27	Joback Method
cpg	349.85	J/mol×K	603.41	Joback Method
cpg	361.25	J/mol×K	636.56	Joback Method
cpg	371.96	J/mol×K	669.71	Joback Method
cpg	382.03	J/mol×K	702.85	Joback Method
cpg	391.47	J/mol×K	736.00	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=C42222060&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