Pentamethylbenzaldehyde

Inchi: InChI=1S/C12H16O/c1-7-8(2)10(4)12(6-13)11(5)9(7)3/h6H,1-5H3
InchiKey: RWOZGGOKRKSHKN-UHFFFAOYSA-N
Formula: C12H16O
SMILES: Cc1c(C)c(C)c(C=O)c(C)c1C
Mol. weight [g/mol]: 176.25
CAS: 17432-38-1

Physical Properties

Property code	Value	Unit	Source
gf	14.90	kJ/mol	Joback Method
hf	-197.41	kJ/mol	Joback Method
hfus	21.22	kJ/mol	Joback Method
hvap	54.61	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.041		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	574.20	K	Joback Method
tc	782.62	K	Joback Method
tf	356.02	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.95	J/mol×K	574.20	Joback Method
cpg	381.77	J/mol×K	608.94	Joback Method
cpg	394.96	J/mol×K	643.67	Joback Method
cpg	407.52	J/mol×K	678.41	Joback Method
cpg	419.46	J/mol×K	713.15	Joback Method
cpg	430.79	J/mol×K	747.88	Joback Method
cpg	441.52	J/mol×K	782.62	Joback Method
dvisc	0.0010025	Pa×s	356.02	Joback Method
dvisc	0.0006945	Pa×s	392.38	Joback Method

dvisc	0.0005120	Pa×s	428.75	Joback Method
dvisc	0.0003959	Pa×s	465.11	Joback Method
dvisc	0.0003178	Pa×s	501.47	Joback Method
dvisc	0.0002628	Pa×s	537.84	Joback Method
dvisc	0.0002226	Pa×s	574.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17432381&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
dvisc:	Dynamic viscosity
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