«alpha»-Methylbenzeneacetaldehyde

Inchi: InChI=1S/C9H10O/c1-8(7-10)9-5-3-2-4-6-9/h2-8H,1H3
InchiKey: IQVAERDLDAZARL-UHFFFAOYSA-N
Formula: C9H10O
SMILES: CC(C=O)c1ccccc1
Mol. weight [g/mol]: 134.18

Physical Properties

Property code	Value	Unit	Source
af	0.3578		Cheméo Relay (1.0)
gf	35.35	kJ/mol	Joback Method
hf	-80.74	kJ/mol	Cheméo Relay (1.0)
hfus	11.87	kJ/mol	Joback Method
hvap	53.93	kJ/mol	Cheméo Relay (1.0)
ie	8.66	eV	Cheméo Relay (1.0)
log10ws	-1.57		Cheméo Relay (1.0)
logp	1.989		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
ripol	1314.00		NIST Webbook
ripol	1314.00		NIST Webbook
tb	470.95	K	Cheméo Relay (1.0)
tc	700.46	K	Cheméo Relay (1.0)
tf	270.59	K	Cheméo Relay (1.0)
vc	0.409	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.06	J/mol×K	480.22	Joback Method
cpg	248.02	J/mol×K	516.50	Joback Method
cpg	260.17	J/mol×K	552.79	Joback Method
cpg	271.54	J/mol×K	589.07	Joback Method
cpg	282.17	J/mol×K	625.36	Joback Method
cpg	292.08	J/mol×K	661.64	Joback Method

cpg	301.32	J/mol×K	697.92	Joback Method
dvisc	0.0048271	Pa×s	244.61	Joback Method
dvisc	0.0021603	Pa×s	283.88	Joback Method
dvisc	0.0011754	Pa×s	323.15	Joback Method
dvisc	0.0007297	Pa×s	362.41	Joback Method
dvisc	0.0004973	Pa×s	401.68	Joback Method
dvisc	0.0003628	Pa×s	440.95	Joback Method
dvisc	0.0002787	Pa×s	480.22	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R633453&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume