Tolualdehyde

Other names: Tolyl aldehyde
Inchi: InChI=1S/C8H8O/c1-7-2-4-8(6-9)5-3-7/h2-6H,1H3
InchiKey: FXLOVSHXALFLKQ-UHFFFAOYSA-N
Formula: C8H8O
SMILES: Cc1ccc(C=O)cc1
Mol. weight [g/mol]: 120.15
CAS: 1334-78-7

Physical Properties

Property code	Value	Unit	Source
gf	19.74	kJ/mol	Joback Method
hf	-68.97	kJ/mol	Joback Method
hfus	12.42	kJ/mol	Joback Method
hvap	43.06	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.808		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1068.00		NIST Webbook
rinpol	1068.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1623.00		NIST Webbook
tb	462.76	K	Joback Method
tc	679.96	K	Joback Method
tf	260.86	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.28	J/mol×K	462.76	Joback Method
cpg	205.24	J/mol×K	498.96	Joback Method
cpg	215.55	J/mol×K	535.16	Joback Method
cpg	225.25	J/mol×K	571.36	Joback Method

cpg	234.35	J/mol×K	607.56	Joback Method
cpg	242.88	J/mol×K	643.76	Joback Method
cpg	250.87	J/mol×K	679.96	Joback Method
dvisc	0.0022848	Pa×s	260.86	Joback Method
dvisc	0.0013282	Pa×s	294.51	Joback Method
dvisc	0.0008630	Pa×s	328.16	Joback Method
dvisc	0.0006075	Pa×s	361.81	Joback Method
dvisc	0.0004540	Pa×s	395.46	Joback Method
dvisc	0.0003551	Pa×s	429.11	Joback Method
dvisc	0.0002879	Pa×s	462.76	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1334787&Units=SI

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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume