Benzaldehyde, 2,4,5-trimethyl-

Other names:	Duraldehyde
	Durylaldehyde
	2,4,5-Trimethylbenzaldehyde
Inchi:	InChI=1S/C10H12O/c1-7-4-9(3)10(6-11)5-8(7)2/h4-6H,1-3H3
InchiKey:	LROJZZICACKNJL-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	Cc1cc(C)c(C=O)cc1C
Mol. weight [g/mol]:	148.20
CAS:	5779-72-6

Physical Properties

Property code	Value	Unit	Source
gf	17.32	kJ/mol	Joback Method
hf	-133.19	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	48.84	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.424		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1376.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1357.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1901.00		NIST Webbook
tb	518.48	K	Joback Method
tc	731.53	K	Joback Method
tf	308.44	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.66	J/mol×K	518.48	Joback Method
cpg	290.15	J/mol×K	553.99	Joback Method
cpg	302.00	J/mol×K	589.50	Joback Method
cpg	313.24	J/mol×K	625.00	Joback Method
cpg	323.88	J/mol×K	660.51	Joback Method
cpg	333.94	J/mol×K	696.02	Joback Method
cpg	343.43	J/mol×K	731.53	Joback Method
dvisc	0.0014505	Pa×s	308.44	Joback Method
dvisc	0.0009364	Pa×s	343.45	Joback Method
dvisc	0.0006555	Pa×s	378.45	Joback Method
dvisc	0.0004874	Pa×s	413.46	Joback Method
dvisc	0.0003796	Pa×s	448.47	Joback Method
dvisc	0.0003065	Pa×s	483.47	Joback Method
dvisc	0.0002548	Pa×s	518.48	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5779726&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
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