Benzenebutanal, «gamma»,4-dimethyl-

Other names: 4-(p-Tolyl)pentanal
Inchi: InChI=1S/C12H16O/c1-10-5-7-12(8-6-10)11(2)4-3-9-13/h5-9,11H,3-4H2,1-2H3
InchiKey: XPYKOJLMORBJQP-UHFFFAOYSA-N
Formula: C12H16O
SMILES: Cc1ccc(C(C)CCC=O)cc1
Mol. weight [g/mol]: 176.25
CAS: 4895-19-6

Physical Properties

Property code	Value	Unit	Source
gf	50.98	kJ/mol	Joback Method
hf	-156.81	kJ/mol	Joback Method
hfus	19.25	kJ/mol	Joback Method
hvap	51.58	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.078		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1406.40		NIST Webbook
rinpol	1406.40		NIST Webbook
tb	553.84	K	Joback Method
tc	762.52	K	Joback Method
tf	290.94	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.33	J/mol×K	553.84	Joback Method
cpg	437.35	J/mol×K	727.74	Joback Method
cpg	425.36	J/mol×K	692.96	Joback Method
cpg	412.59	J/mol×K	658.18	Joback Method
cpg	399.02	J/mol×K	623.40	Joback Method
cpg	384.61	J/mol×K	588.62	Joback Method

cpg	448.60	J/mol×K	762.52	Joback Method
dvisc	0.0002268	Pa×s	553.84	Joback Method
dvisc	0.0002931	Pa×s	510.02	Joback Method
dvisc	0.0003974	Pa×s	466.21	Joback Method
dvisc	0.0005741	Pa×s	422.39	Joback Method
dvisc	0.0009031	Pa×s	378.57	Joback Method
dvisc	0.0015993	Pa×s	334.76	Joback Method
dvisc	0.0033642	Pa×s	290.94	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=C4895196&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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