

trans-4-Methoxycinnamaldehyde

Other names:	4-Methoxycinnamaldehyde (E)-3-(4-Methoxyphenyl)acrylaldehyde
Inchi:	InChI=1S/C10H10O2/c1-12-10-6-4-9(5-7-10)3-2-8-11/h2-8H,1H3/b3-2+
InchiKey:	AXCXHFKZHDEKTP-NSCUHNMNSA-N
Formula:	C10H10O2
SMILES:	COc1ccc(C=CC=O)cc1
Mol. weight [g/mol]:	162.19
CAS:	24680-50-0

Physical Properties

Property code	Value	Unit	Source
gf	11.80	kJ/mol	Joback Method
hf	-125.25	kJ/mol	Joback Method
hfus	18.99	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	1.907		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	1569.80		NIST Webbook
rinpol	1569.80		NIST Webbook
tb	535.10	K	Joback Method
tc	753.45	K	Joback Method
tf	300.55	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.74	J/mol×K	535.10	Joback Method
cpg	295.09	J/mol×K	571.49	Joback Method
cpg	306.70	J/mol×K	607.88	Joback Method
cpg	317.59	J/mol×K	644.27	Joback Method
cpg	327.80	J/mol×K	680.66	Joback Method

cpg	337.35	J/mol×K	717.05	Joback Method
cpg	346.28	J/mol×K	753.45	Joback Method
dvisc	0.0017915	Pa×s	300.55	Joback Method
dvisc	0.0009990	Pa×s	339.64	Joback Method
dvisc	0.0006285	Pa×s	378.73	Joback Method
dvisc	0.0004312	Pa×s	417.82	Joback Method
dvisc	0.0003155	Pa×s	456.92	Joback Method
dvisc	0.0002425	Pa×s	496.01	Joback Method
dvisc	0.0001937	Pa×s	535.10	Joback Method

Sources

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=C24680500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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