

(E)-3-Methylcinnamaldehyde

Inchi:	InChI=1S/C10H10O/c1-9-4-2-5-10(8-9)6-3-7-11/h2-8H,1H3/b6-3+
InchiKey:	SJLLZWMNPJCLBC-ZZXKWWIFSA-N
Formula:	C10H10O
SMILES:	<chem>Cc1cccc(C=CC=O)c1</chem>
Mol. weight [g/mol]:	146.19

Physical Properties

Property code	Value	Unit	Source
gf	116.80	kJ/mol	Joback Method
hf	6.97	kJ/mol	Joback Method
hfus	17.80	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.207		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
tb	512.68	K	Joback Method
tc	733.50	K	Joback Method
tf	278.32	K	Joback Method
vc	0.484	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.86	J/mol×K	512.68	Joback Method
cpg	315.28	J/mol×K	696.70	Joback Method
cpg	305.68	J/mol×K	659.89	Joback Method
cpg	295.38	J/mol×K	623.09	Joback Method
cpg	284.34	J/mol×K	586.29	Joback Method
cpg	272.52	J/mol×K	549.48	Joback Method
cpg	324.23	J/mol×K	733.50	Joback Method
dvisc	0.0002293	Paxs	512.68	Joback Method

dvisc	0.0002874	Paxs	473.62	Joback Method
dvisc	0.0003751	Paxs	434.56	Joback Method
dvisc	0.0005159	Paxs	395.50	Joback Method
dvisc	0.0007611	Paxs	356.44	Joback Method
dvisc	0.0012355	Paxs	317.38	Joback Method
dvisc	0.0022976	Paxs	278.32	Joback Method

Sources

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=R396857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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