

3-Methoxycinnamaldehyde

Inchi:	InChI=1S/C10H10O2/c1-12-10-6-2-4-9(8-10)5-3-7-11/h2-8H,1H3/b5-3+
InchiKey:	XHYAQFCRAQUBTD-HWKANZROSA-N
Formula:	C10H10O2
SMILES:	COc1cccc(C=CC=O)c1
Mol. weight [g/mol]:	162.19
CAS:	56578-36-0

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
mvol	131.140	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
ripol	2565.00		NIST Webbook
tb	535.10	K	Joback Method
tc	753.45	K	Joback Method
tf	300.55	K	Joback Method
vc	0.502	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.74	J/molxK	535.10	Joback Method
cpg	295.09	J/molxK	571.49	Joback Method
cpg	306.70	J/molxK	607.88	Joback Method
cpg	317.59	J/molxK	644.27	Joback Method
cpg	327.80	J/molxK	680.66	Joback Method
cpg	337.35	J/molxK	717.05	Joback Method
cpg	346.28	J/molxK	753.45	Joback Method
dvisc	0.0017915	Paxs	300.55	Joback Method

dvisc	0.0009990	Paxs	339.64	Joback Method
dvisc	0.0006285	Paxs	378.73	Joback Method
dvisc	0.0004312	Paxs	417.82	Joback Method
dvisc	0.0003155	Paxs	456.92	Joback Method
dvisc	0.0002425	Paxs	496.01	Joback Method
dvisc	0.0001937	Paxs	535.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56578360&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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