(E)-3-(2-Methoxyphenyl)-2-propenoic acid

Other names: 2-Propenoic acid, 3-(2-methoxyphenyl)-, (E)-
(E)-o-methoxycinnamic acid
Inchi: InChI=1S/C10H10O3/c1-13-9-5-3-2-4-8(9)6-7-10(11)12/h2-7H,1H3,(H,11,12)/b7-6+
InchiKey: FEGVSPGUHMGGBO-VOTSOKGWSA-N
Formula: C10H10O3
SMILES: COc1ccccc1C=CC(=O)O
Mol. weight [g/mol]: 178.18
CAS: 1011-54-7

Physical Properties

Property code	Value	Unit	Source
gf	-154.42	kJ/mol	Joback Method
hf	-304.48	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hsub	128.80 ± 0.60	kJ/mol	NIST Webbook
hvap	66.59	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
log10ws	-1.93		Crippen Method
logp	1.793		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	632.49	K	Joback Method
tc	839.79	K	Joback Method
tf	369.30	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.56	J/mol×K	632.49	Joback Method
cpg	338.85	J/mol×K	667.04	Joback Method
cpg	348.51	J/mol×K	701.59	Joback Method
cpg	357.56	J/mol×K	736.14	Joback Method
cpg	366.02	J/mol×K	770.69	Joback Method

cpg	373.93	J/mol×K	805.24	Joback Method
cpg	381.31	J/mol×K	839.79	Joback Method
dvisc	0.0023160	Pa×s	369.30	Joback Method
dvisc	0.0008973	Pa×s	413.17	Joback Method
dvisc	0.0004170	Pa×s	457.03	Joback Method
dvisc	0.0002217	Pa×s	500.89	Joback Method
dvisc	0.0001304	Pa×s	544.76	Joback Method
dvisc	0.0000831	Pa×s	588.62	Joback Method
dvisc	0.0000563	Pa×s	632.49	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=C1011547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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