

(Z)-Ethyl 3-(4-methoxyphenyl)acrylate

Inchi:	InChI=1S/C12H14O3/c1-3-15-12(13)9-6-10-4-7-11(14-2)8-5-10/h4-9H,3H2,1-2H3/b9-6-
InchiKey:	DHNGCHLFKUPGPX-TWGQIWQCSA-N
Formula:	C12H14O3
SMILES:	CCOC(=O)C=Cc1ccc(OC)cc1
Mol. weight [g/mol]:	206.24
CAS:	51507-22-3

Physical Properties

Property code	Value	Unit	Source
gf	-105.76	kJ/mol	Joback Method
hf	-325.75	kJ/mol	Joback Method
hfus	24.67	kJ/mol	Joback Method
hvap	56.77	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.272		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1669.70		NIST Webbook
tb	608.49	K	Joback Method
tc	821.95	K	Joback Method
tf	353.25	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.77	J/mol×K	608.49	Joback Method
cpg	412.88	J/mol×K	644.07	Joback Method
cpg	426.17	J/mol×K	679.64	Joback Method
cpg	438.68	J/mol×K	715.22	Joback Method
cpg	450.41	J/mol×K	750.80	Joback Method
cpg	461.38	J/mol×K	786.38	Joback Method
cpg	471.62	J/mol×K	821.95	Joback Method
dvisc	0.0011684	Pa×s	353.25	Joback Method

dvisc	0.0006576	Pa×s	395.79	Joback Method
dvisc	0.0004138	Pa×s	438.33	Joback Method
dvisc	0.0002826	Pa×s	480.87	Joback Method
dvisc	0.0002054	Pa×s	523.41	Joback Method
dvisc	0.0001566	Pa×s	565.95	Joback Method
dvisc	0.0001240	Pa×s	608.49	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=C51507223&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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