

2-Methylpropionic acid, 4-methoxyphenyl ester

Inchi:	InChI=1S/C11H14O3/c1-8(2)11(12)14-10-6-4-9(13-3)5-7-10/h4-8H,1-3H3
InchiKey:	WKQWJJFHPKIPDM-UHFFFAOYSA-N
Formula:	C11H14O3
SMILES:	COc1ccc(OC(=O)C(C)C)cc1
Mol. weight [g/mol]:	194.23

Physical Properties

Property code	Value	Unit	Source
gf	-196.84	kJ/mol	Joback Method
hf	-427.61	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	54.20	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.257		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinsol	1431.00		NIST Webbook
tb	581.01	K	Joback Method
tc	793.47	K	Joback Method
tf	332.06	K	Joback Method
vc	0.580	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.20	J/molxK	581.01	Joback Method
cpg	385.45	J/molxK	616.42	Joback Method
cpg	398.95	J/molxK	651.83	Joback Method
cpg	411.70	J/molxK	687.24	Joback Method
cpg	423.70	J/molxK	722.65	Joback Method
cpg	434.96	J/molxK	758.06	Joback Method
cpg	445.46	J/molxK	793.47	Joback Method
dvisc	0.0016320	Paxs	332.06	Joback Method
dvisc	0.0008770	Paxs	373.55	Joback Method

dvisc	0.0005336	Paxs	415.04	Joback Method
dvisc	0.0003554	Paxs	456.53	Joback Method
dvisc	0.0002532	Paxs	498.03	Joback Method
dvisc	0.0001901	Paxs	539.52	Joback Method
dvisc	0.0001487	Paxs	581.01	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308017&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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