

Phenylacetic acid, 4-methoxyphenyl ester

Inchi:	InChI=1S/C15H14O3/c1-17-13-7-9-14(10-8-13)18-15(16)11-12-5-3-2-4-6-12/h2-10H,11H
InchiKey:	QLPZFSTUQGHNJ-UHFFFAOYSA-N
Formula:	C15H14O3
SMILES:	COc1ccc(OC(=O)Cc2ccccc2)cc1
Mol. weight [g/mol]:	242.27

Physical Properties

Property code	Value	Unit	Source
gf	-48.31	kJ/mol	Joback Method
hf	-268.36	kJ/mol	Joback Method
hfus	26.27	kJ/mol	Joback Method
hvap	65.76	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.843		Crippen Method
mvol	188.000	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1954.00		NIST Webbook
tb	699.65	K	Joback Method
tc	934.64	K	Joback Method
tf	418.56	K	Joback Method
vc	0.702	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.63	J/molxK	699.65	Joback Method
cpg	506.76	J/molxK	738.81	Joback Method
cpg	520.73	J/molxK	777.98	Joback Method
cpg	533.56	J/molxK	817.14	Joback Method
cpg	545.27	J/molxK	856.31	Joback Method
cpg	555.89	J/molxK	895.47	Joback Method
cpg	565.45	J/molxK	934.64	Joback Method
dvisc	0.0009037	Paxs	418.56	Joback Method
dvisc	0.0005287	Paxs	465.41	Joback Method

dvisc	0.0003412	Paxs	512.26	Joback Method
dvisc	0.0002370	Paxs	559.11	Joback Method
dvisc	0.0001741	Paxs	605.95	Joback Method
dvisc	0.0001337	Paxs	652.80	Joback Method
dvisc	0.0001064	Paxs	699.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307533&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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