

Octanoic acid, 4-methoxyphenyl ester

Inchi:	InChI=1S/C15H22O3/c1-3-4-5-6-7-8-15(16)18-14-11-9-13(17-2)10-12-14/h9-12H,3-8H2,
InchiKey:	ZYRMFAWNABLGKS-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	CCCCCCCC(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]:	250.33

Physical Properties

Property code	Value	Unit	Source
gf	-160.72	kJ/mol	Joback Method
hf	-504.89	kJ/mol	Joback Method
hfus	32.23	kJ/mol	Joback Method
hvap	63.49	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.961		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpola	1899.00		NIST Webbook
tb	672.97	K	Joback Method
tc	869.94	K	Joback Method
tf	392.14	K	Joback Method
vc	0.809	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.00	J/molxK	672.97	Joback Method
cpg	590.26	J/molxK	705.80	Joback Method
cpg	605.64	J/molxK	738.63	Joback Method
cpg	620.13	J/molxK	771.45	Joback Method
cpg	633.77	J/molxK	804.28	Joback Method
cpg	646.54	J/molxK	837.11	Joback Method
cpg	658.47	J/molxK	869.94	Joback Method
dvisc	0.0010931	Paxs	392.14	Joback Method
dvisc	0.0006017	Paxs	438.95	Joback Method

dvisc	0.0003716	Paxs	485.75	Joback Method
dvisc	0.0002498	Paxs	532.56	Joback Method
dvisc	0.0001790	Paxs	579.36	Joback Method
dvisc	0.0001349	Paxs	626.17	Joback Method
dvisc	0.0001057	Paxs	672.97	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=U307697&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
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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