4-(4-Phenoxyphenyl)butanoic acid methyl ester

Inchi: InChI=1S/C17H18O3/c1-19-17(18)9-5-6-14-10-12-16(13-11-14)20-15-7-3-2-4-8-15/h2-4,

InchiKey: VTGLGZNRGWSTHU-UHFFFAOYSA-N

Formula: C17H18O3

SMILES: COC(=O)CCCc1ccc(Oc2ccccc2)cc1

Mol. weight [g/mol]: 270.32

CAS: 24254-59-9

Physical Properties

Property code	Value	Unit	Source
gf	-31.47	kJ/mol	Joback Method
hf	-309.64	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Joback Method
ie	7.90 ± 0.20	eV	NIST Webbook
log10ws	-4.03		Crippen Method
logp	3.975		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
tb	745.41	K	Joback Method
tc	971.98	K	Joback Method
tf	441.10	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.41	J/mol×K	745.41	Joback Method
cpg	665.49	J/mol×K	934.22	Joback Method
cpg	654.37	J/mol×K	896.46	Joback Method
cpg	642.13	J/mol×K	858.69	Joback Method
cpg	628.74	J/mol×K	820.93	Joback Method
cpg	614.18	J/mol×K	783.17	Joback Method
cpg	675.53	J/mol×K	971.98	Joback Method
dvisc	0.0000844	Pa×s	745.41	Joback Method

dvisc	0.0001070	Pa×s	694.69	Joback Method
dvisc	0.0001407	Pa×s	643.97	Joback Method
dvisc	0.0001939	Pa×s	593.25	Joback Method
dvisc	0.0002838	Pa×s	542.54	Joback Method
dvisc	0.0004493	Pa×s	491.82	Joback Method
dvisc	0.0007907	Pa×s	441.10	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=C24254599&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
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