Phenylacetic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C16H16O2/c1-12-8-13(2)10-15(9-12)18-16(17)11-14-6-4-3-5-7-14/h3-10H,11H
InchiKey: IDUWQVRMDQHGCN-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: Cc1cc(C)cc(OC(=O)Cc2ccccc2)c1
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	55.48	kJ/mol	Joback Method
hf	-168.25	kJ/mol	Joback Method
hfus	27.29	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.452		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	1888.00		NIST Webbook
rinpol	1888.00		NIST Webbook
tb	705.09	K	Joback Method
tc	939.69	K	Joback Method
tf	420.12	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.05	J/mol×K	705.09	Joback Method
cpg	584.75	J/mol×K	900.59	Joback Method
cpg	573.40	J/mol×K	861.49	Joback Method
cpg	560.99	J/mol×K	822.39	Joback Method
cpg	547.49	J/mol×K	783.29	Joback Method
cpg	532.86	J/mol×K	744.19	Joback Method
cpg	595.10	J/mol×K	939.69	Joback Method
dvisc	0.0001219	Pa×s	705.09	Joback Method

dvisc	0.0001519	Pa×s	657.59	Joback Method
dvisc	0.0001959	Pa×s	610.10	Joback Method
dvisc	0.0002638	Pa×s	562.61	Joback Method
dvisc	0.0003752	Pa×s	515.11	Joback Method
dvisc	0.0005733	Pa×s	467.62	Joback Method
dvisc	0.0009640	Pa×s	420.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307532&Units=SI
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

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