3-Cyclopentylpropionic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C16H22O2/c1-12-9-13(2)11-15(10-12)18-16(17)8-7-14-5-3-4-6-14/h9-11,14H,3

InchiKey: OKDQBRBJEFQPGL-UHFFFAOYSA-N

Formula: C16H22O2

SMILES: Cc1cc(C)cc(OC(=O)CCC2CCCC2)c1

Mol. weight [g/mol]: 246.34

Physical Properties

Property code	Value	Unit	Source
gf	-20.38	kJ/mol	Joback Method
hf	-344.30	kJ/mol	Joback Method
hfus	27.18	kJ/mol	Joback Method
hvap	64.22	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.179		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1902.00		NIST Webbook
tb	693.69	K	Joback Method
tc	914.87	K	Joback Method
tf	404.60	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.10	J/mol×K	693.69	Joback Method
cpg	608.87	J/mol×K	730.55	Joback Method
cpg	626.40	J/mol×K	767.42	Joback Method
cpg	642.74	J/mol×K	804.28	Joback Method
cpg	657.91	J/mol×K	841.14	Joback Method
cpg	671.97	J/mol×K	878.00	Joback Method
cpg	684.94	J/mol×K	914.87	Joback Method
dvisc	0.0014044	Pa×s	404.60	Joback Method
dvisc	0.0008240	Pa×s	452.78	Joback Method

dvisc	0.0005357	Pa×s	500.96	Joback Method
dvisc	0.0003756	Pa×s	549.14	Joback Method
dvisc	0.0002789	Pa×s	597.33	Joback Method
dvisc	0.0002165	Pa×s	645.51	Joback Method
dvisc	0.0001741	Pa×s	693.69	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=U307132&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