3-Cyclopentylpropionic acid, 3-ethylphenyl ester

Inchi: InChI=1S/C16H22O2/c1-2-13-8-5-9-15(12-13)18-16(17)11-10-14-6-3-4-7-14/h5,8-9,12,14

InchiKey: UHLFJGFCIVLDBM-UHFFFAOYSA-N

Formula: C16H22O2

SMILES: CCc1cccc(OC(=O)CCC2CCCC2)c1

Mol. weight [g/mol]: 246.34

Physical Properties

Property code	Value	Unit	Source
gf	-10.75	kJ/mol	Joback Method
hf	-332.83	kJ/mol	Joback Method
hfus	27.57	kJ/mol	Joback Method
hvap	63.56	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.125		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	1978.00		NIST Webbook
tb	688.71	K	Joback Method
tc	909.05	K	Joback Method
tf	392.08	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.47	J/mol×K	688.71	Joback Method
cpg	672.98	J/mol×K	872.33	Joback Method
cpg	658.83	J/mol×K	835.61	Joback Method
cpg	643.55	J/mol×K	798.88	Joback Method
cpg	627.09	J/mol×K	762.16	Joback Method
cpg	609.42	J/mol×K	725.43	Joback Method
cpg	686.04	J/mol×K	909.05	Joback Method
dvisc	0.0001743	Pa×s	688.71	Joback Method
dvisc	0.0002202	Pa×s	639.27	Joback Method

dvisc	0.0002891	Pa×s	589.83	Joback Method
dvisc	0.0003991	Pa×s	540.39	Joback Method
dvisc	0.0005879	Pa×s	490.96	Joback Method
dvisc	0.0009444	Pa×s	441.52	Joback Method
dvisc	0.0017097	Pa×s	392.08	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=U354056&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