

3-Cyclopentylpropionic acid, 2,3-dimethylphenyl ester

Inchi:	InChI=1S/C16H22O2/c1-12-6-5-9-15(13(12)2)18-16(17)11-10-14-7-3-4-8-14/h5-6,9,14H,
InchiKey:	WADHQKLYUCHLGE-UHFFFAOYSA-N
Formula:	C16H22O2
SMILES:	Cc1cccc(OC(=O)CCC2CCCC2)c1C
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
rinsol	2007.00		NIST Webbook
tb	693.69	K	Joback Method
tc	914.87	K	Joback Method
tf	404.60	K	Joback Method
vc	0.788	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0005357	Paxs	500.96	Joback Method
dvisc	0.0003756	Paxs	549.14	Joback Method
dvisc	0.0002789	Paxs	597.33	Joback Method
dvisc	0.0002165	Paxs	645.51	Joback Method
dvisc	0.0001741	Paxs	693.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354057&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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