

1-(P-METHOXYPHENYL)-1-CYCLOHEXANECARB

Other names:

1-(4-methoxyphenyl)cyclohexane-1-carboxylic acid
Cyclohexanecarboxylic acid, 1-(4-methoxyphenyl)-

Inchi: InChI=1S/C14H18O3/c1-17-12-7-5-11(6-8-12)14(13(15)16)9-3-2-4-10-14/h5-8H,2-4,9-10

InchiKey: JKJAJSWMKTWWJS-UHFFFAOYSA-N

Formula: C14H18O3

SMILES: COc1ccc(C2(C(=O)O)CCCCC2)cc1

Mol. weight [g/mol]: 234.30

Physical Properties

Property code	Value	Unit	Source
hf	-488.11	kJ/mol	Cheméo Relay (1.0)
hfus	18.08	kJ/mol	Joback Method
hvap	90.59	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	Cheméo Relay (1.0)
log10ws	-3.56		Cheméo Relay (1.0)
logp	2.982		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
tb	623.49	K	Cheméo Relay (1.0)
tf	442.35	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.54	J/mol×K	739.64	Joback Method
cpg	557.08	J/mol×K	777.16	Joback Method
cpg	571.89	J/mol×K	814.67	Joback Method
cpg	586.08	J/mol×K	852.19	Joback Method
cpg	599.81	J/mol×K	889.70	Joback Method
cpg	613.18	J/mol×K	927.22	Joback Method
cpg	626.34	J/mol×K	964.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7469832&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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