

1,2-Cyclohexanedicarboxylic acid, 4-methoxyphenyl propyl ester

Inchi:	InChI=1S/C18H24O5/c1-3-12-22-17(19)15-6-4-5-7-16(15)18(20)23-14-10-8-13(21-2)9-1
InchiKey:	RLPBPLYCLFJANK-UHFFFAOYSA-N
Formula:	C18H24O5
SMILES:	CCCOC(=O)C1CCCCC1C(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]:	320.38

Physical Properties

Property code	Value	Unit	Source
gf	-352.64	kJ/mol	Joback Method
hf	-777.63	kJ/mol	Joback Method
hfus	35.70	kJ/mol	Joback Method
hvap	79.44	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.360		Crippen Method
mcvol	250.610	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2415.00		NIST Webbook
tb	832.78	K	Joback Method
tc	1054.40	K	Joback Method
tf	501.25	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.40	J/molxK	832.78	Joback Method
cpg	856.45	J/molxK	1017.47	Joback Method
cpg	845.94	J/molxK	980.53	Joback Method
cpg	833.88	J/molxK	943.59	Joback Method
cpg	820.27	J/molxK	906.65	Joback Method
cpg	805.11	J/molxK	869.72	Joback Method
cpg	865.42	J/molxK	1054.40	Joback Method
dvisc	0.0000726	Paxs	832.78	Joback Method
dvisc	0.0000915	Paxs	777.52	Joback Method

dvisc	0.0001197	Paxs	722.27	Joback Method
dvisc	0.0001635	Paxs	667.01	Joback Method
dvisc	0.0002364	Paxs	611.76	Joback Method
dvisc	0.0003678	Paxs	556.50	Joback Method
dvisc	0.0006307	Paxs	501.25	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339667&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

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