

1,2-Cyclohexanedicarboxylic acid, 2,6-dimethoxyphenyl ethyl ester

Inchi: InChI=1S/C18H24O6/c1-4-23-17(19)12-8-5-6-9-13(12)18(20)24-16-14(21-2)10-7-11-15(1)
InchiKey: GQZIIZYLEUIBCD-UHFFFAOYSA-N
Formula: C18H24O6
SMILES: CCOC(=O)C1CCCCC1C(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	-467.27	kJ/mol	Joback Method
hf	-921.32	kJ/mol	Joback Method
hfus	36.49	kJ/mol	Joback Method
hvap	82.51	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.979		Crippen Method
mcvol	256.480	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
tb	860.18	K	Joback Method
tc	1081.40	K	Joback Method
tf	536.00	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.22	J/mol×K	860.18	Joback Method
cpg	831.96	J/mol×K	897.05	Joback Method
cpg	846.05	J/mol×K	933.92	Joback Method
cpg	858.48	J/mol×K	970.79	Joback Method
cpg	869.22	J/mol×K	1007.66	Joback Method
cpg	878.25	J/mol×K	1044.53	Joback Method
cpg	885.54	J/mol×K	1081.40	Joback Method
dvisc	0.0003969	Pa×s	536.00	Joback Method

dvisc	0.0002462	Pa×s	590.03	Joback Method
dvisc	0.0001655	Pa×s	644.06	Joback Method
dvisc	0.0001183	Pa×s	698.09	Joback Method
dvisc	0.0000888	Pa×s	752.12	Joback Method
dvisc	0.0000692	Pa×s	806.15	Joback Method
dvisc	0.0000557	Pa×s	860.18	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=U339929&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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