

cis-Cyclohex-4-en-1,2-dicarboxylic acid, ethyl phenethyl ester

Inchi:	InChI=1S/C18H22O4/c1-2-21-17(19)15-10-6-7-11-16(15)18(20)22-13-12-14-8-4-3-5-9-14
InchiKey:	MSJQIKZXODCXGU-UHFFFAOYSA-N
Formula:	C18H22O4
SMILES:	CCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	302.36

Physical Properties

Property code	Value	Unit	Source
gf	-208.05	kJ/mol	Joback Method
hf	-576.16	kJ/mol	Joback Method
hfus	36.12	kJ/mol	Joback Method
hvap	76.66	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.918		Crippen Method
mcvol	240.440	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
rinsol	2230.00		NIST Webbook
tb	804.54	K	Joback Method
tc	1028.55	K	Joback Method
tf	467.26	K	Joback Method
vc	0.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.89	J/molxK	804.54	Joback Method
cpg	749.66	J/molxK	841.87	Joback Method
cpg	764.98	J/molxK	879.21	Joback Method
cpg	778.88	J/molxK	916.54	Joback Method
cpg	791.37	J/molxK	953.88	Joback Method
cpg	802.49	J/molxK	991.21	Joback Method
cpg	812.27	J/molxK	1028.55	Joback Method
dvisc	0.0010039	Paxs	467.26	Joback Method
dvisc	0.0005579	Paxs	523.47	Joback Method

dvisc	0.0003475	Paxs	579.69	Joback Method
dvisc	0.0002353	Paxs	635.90	Joback Method
dvisc	0.0001698	Paxs	692.11	Joback Method
dvisc	0.0001286	Paxs	748.33	Joback Method
dvisc	0.0001013	Paxs	804.54	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=U382787&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

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