

1,2-Cyclohexanedicarboxylic acid, ethyl pentyl ester

Inchi:	InChI=1S/C15H26O4/c1-3-5-8-11-19-15(17)13-10-7-6-9-12(13)14(16)18-4-2/h12-13H,3-
InchiKey:	PCPOYRXAOUSZIA-UHFFFAOYSA-N
Formula:	C15H26O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OCC
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-375.68	kJ/mol	Joback Method
hf	-808.55	kJ/mol	Joback Method
hfus	33.09	kJ/mol	Joback Method
hvap	67.42	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.089		Crippen Method
mcvol	226.230	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1848.00		NIST Webbook
tb	710.06	K	Joback Method
tc	907.67	K	Joback Method
tf	406.27	K	Joback Method
vc	0.856	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.22	J/molxK	710.06	Joback Method
cpg	756.04	J/molxK	874.74	Joback Method
cpg	741.88	J/molxK	841.80	Joback Method
cpg	726.62	J/molxK	808.87	Joback Method
cpg	710.26	J/molxK	775.93	Joback Method
cpg	692.80	J/molxK	743.00	Joback Method
cpg	769.11	J/molxK	907.67	Joback Method
dvisc	0.0001354	Paxs	710.06	Joback Method
dvisc	0.0001743	Paxs	659.43	Joback Method

dvisc	0.0002340	Paxs	608.80	Joback Method
dvisc	0.0003314	Paxs	558.16	Joback Method
dvisc	0.0005032	Paxs	507.53	Joback Method
dvisc	0.0008379	Paxs	456.90	Joback Method
dvisc	0.0015847	Paxs	406.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339464&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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