

1,2-Cyclohexanedicarboxylic acid, ethyl furfuryl ester

Inchi:	InChI=1S/C15H24O5/c1-2-18-14(16)12-7-3-4-8-13(12)15(17)20-10-11-6-5-9-19-11/h11-1
InchiKey:	NYSNJRYSWGQEOC-UHFFFAOYSA-N
Formula:	C15H24O5
SMILES:	CCOC(=O)C1CCCCC1C(=O)OCC1CCCO1
Mol. weight [g/mol]:	284.35

Physical Properties

Property code	Value	Unit	Source
gf	-425.25	kJ/mol	Joback Method
hf	-880.07	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	72.18	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.078		Crippen Method
mvol	221.240	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	752.29	K	Joback Method
tc	970.77	K	Joback Method
tf	443.74	K	Joback Method
vc	0.818	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.36	J/molxK	752.29	Joback Method
cpg	719.57	J/molxK	788.70	Joback Method
cpg	737.33	J/molxK	825.12	Joback Method
cpg	753.64	J/molxK	861.53	Joback Method
cpg	768.53	J/molxK	897.94	Joback Method
cpg	782.00	J/molxK	934.35	Joback Method
cpg	794.08	J/molxK	970.77	Joback Method
dvisc	0.0017432	Paxs	443.74	Joback Method

dvisc	0.0009770	Paxs	495.17	Joback Method
dvisc	0.0006106	Paxs	546.59	Joback Method
dvisc	0.0004138	Paxs	598.01	Joback Method
dvisc	0.0002982	Paxs	649.44	Joback Method
dvisc	0.0002255	Paxs	700.87	Joback Method
dvisc	0.0001772	Paxs	752.29	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=U339896&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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