

1,2-Cyclohexanedicarboxylic acid, ethyl isobutyl ester

Inchi:	InChI=1S/C14H24O4/c1-4-17-13(15)11-7-5-6-8-12(11)14(16)18-9-10(2)3/h10-12H,4-9H2
InchiKey:	QJUUFFMQQPZLBA-UHFFFAOYSA-N
Formula:	C14H24O4
SMILES:	CCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	256.34

Physical Properties

Property code	Value	Unit	Source
gf	-386.54	kJ/mol	Joback Method
hf	-793.19	kJ/mol	Joback Method
hfus	26.97	kJ/mol	Joback Method
hvap	64.80	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.555		Crippen Method
mcvol	212.140	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	1699.00		NIST Webbook
rinpol	1699.00		NIST Webbook
tb	686.74	K	Joback Method
tc	889.72	K	Joback Method
tf	380.00	K	Joback Method
vc	0.793	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.58	J/molxK	686.74	Joback Method
cpg	637.25	J/molxK	720.57	Joback Method
cpg	654.81	J/molxK	754.40	Joback Method
cpg	671.25	J/molxK	788.23	Joback Method
cpg	686.57	J/molxK	822.06	Joback Method
cpg	700.78	J/molxK	855.89	Joback Method
cpg	713.89	J/molxK	889.72	Joback Method
dvisc	0.0020571	Paxs	380.00	Joback Method

dvisc	0.0010100	Paxs	431.12	Joback Method
dvisc	0.0005766	Paxs	482.25	Joback Method
dvisc	0.0003665	Paxs	533.37	Joback Method
dvisc	0.0002522	Paxs	584.49	Joback Method
dvisc	0.0001843	Paxs	635.62	Joback Method
dvisc	0.0001411	Paxs	686.74	Joback Method

Sources

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=U339422&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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